

CFD Modeling of Biomass Gasification
Using a Circulating Fluidized Bed Reactor

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis, except where is noted. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

Biomass, as a renewable energy resource, can be utilized to generate chemicals, heat, and electricity. Compared with biomass combustion, biomass gasification is more eco-friendly because it generates less amount of green gas (CO_2) and other polluting gases (NO_x and SO_2).

This research is focused on biomass gasification using a circulating fluidized bed. In the gasifier, fully fluidized biomass particles react with water vapor and air to generate syngas (CO and H_2). A comprehensive model, consisting of three modules, hydrodynamics, mass transfer and energy transfer modules, is built to simulate this process using ANSYS Fluent software and C programming language. In the hydrodynamics module, the k-epsilon turbulence equations are coupled with the fluctuating energy equation to simulate gas-particle interaction in the turbulent flows occurring in the riser. In the mass transfer and energy transfer modules, heat transfer and mass transfer in turbulent flows are simulated to solve for the profiles of temperature and species concentration in the gasifier. The impacts of thermal radiation, water gas shift reaction (WGS), equivalence ratio (ER), and char combustion product distribution coefficient are also investigated to gain deeper understanding of biomass gasification process.

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List of Abbreviation

CFB	Circulating Fluidized Bed
CFD	Computational Fluid Dynamics
E-E	Eulerian-Eulerian
EMMS	Energy Minimization Multi-Scale
ER	Equivalence Ratio
RNG	Re-Normalization Group
WGS	Water Gas Shift

Chapter 1

Introduction

1.1 Background

Nowadays, highly developed industries consume enormous amount of fossil fuels. However, as limited natural resources, fossil fuels cannot be re-generated and will be depleted in future; meanwhile, their soaring prices also enforce us to seek for alternative energy resources. Biomass, as a renewable energy source, can be considered as an alternative to match increasing demand from industries [1]. Additionally, some biomass conversion technology such as biomass gasification can also be beneficial in decreasing greenhouse gases emissions [2].

Instead of simply being burned, biomass can be utilized to generate chemicals, electricity, and heat through gasification process. Compared with biomass combustion, biomass gasification has a lower environmental impact due to less greenhouse gas emission [3], and this process can be applied not only to generate power but also to synthesize some chemicals such as ammonia, methanol or higher alcohols [4]. Furthermore, the application of biomass gasification can also conserve the finite fossil energy resources, reduce the dependency on fossil fuels, and enhance energy security [5].

Many types of gasifiers are employed in industry, and are categorized into three groups, fixed bed gasifiers, fluidized bed gasifiers, and entrained flow gasifiers, as shown in Figure 1.

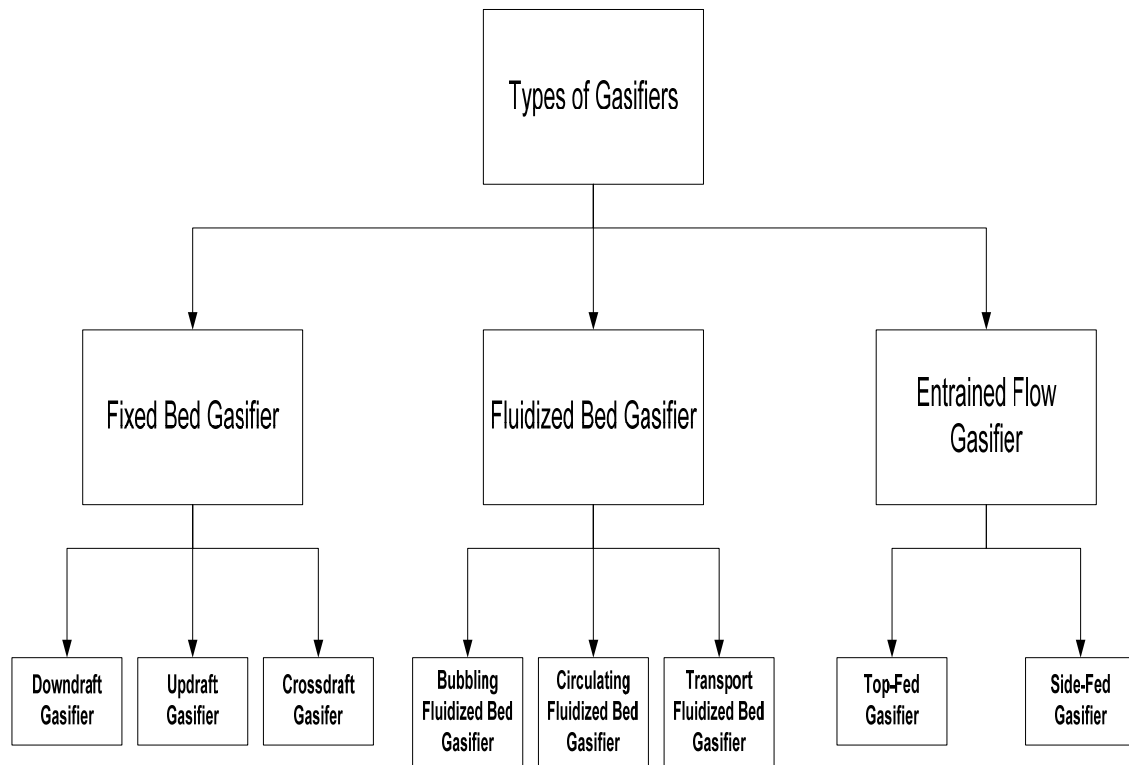


Figure 1: Types of Gasifiers

Fixed bed gasifiers are generally suitable for small scale gasification production and can also be used in some areas such as drying, absorption, and calcinations [6]. However, due to poor mixing of air and solid particles, mass and heat transfer in such gasifiers is less efficient than other types of gasifiers, and longer reaction residence time is required to achieve full conversion of carbonaceous solid fuels.

In a fluidized bed gasifier, solid fuel particles are generally fed at the side of the gasifier while air or oxygen gas enters at the bottom of the gasifier. Solid fuel particles suspend or move up in the gasifier due to the drag force of upward gas flow, acting as a fluid. Since solid fuel particles are fluidized by the gasifying agents, the mixing of gas and solid in fluidized gasifiers are then more thorough than fixed bed gasifiers. Consequently, mass and energy transfer in fluidized gasifier becomes highly efficient.

Figure 2 demonstrates the hydrodynamic transition from a fixed bed to a transport bed. As shown in the figure, in a fixed bed reactor, solid particles reside on the grate where the

air percolates through. Since the gas velocity is very slow, solid particles cannot move and the bed remains in a stationary state.

However, once the gas velocity increases and reaches the “minimum fluidization velocity”, the bed starts to expand. As seen in Figure 2, with further increase in gas velocity, the hydrodynamics of bubbling fluidized bed (BFB) then appears. Bubbles are formed when the gas flows through the bed. Some solid particles are entrained in the rising bubbles, but most of them will be disengaged from the gas stream and eventually fall down to the bed when the bubbles erupt above the solid bed.

When the gas velocity further increases, a regime of fast fluidized bed then starts to form. As displayed in Figure 2, the solid bed does not exist anymore and all of solid particles are suspended in the gas due to high gas superficial velocity (3.5-5.5 m/s). Some particles may collide and stick to each other to form clusters. Bigger particles and clusters may remain near the bottom, while smaller particles and clusters may move up to higher locations. In industry, a gasifier with a fast fluidized bed is generally called circulating fluidized bed (CFB) gasifier and the term “circulating” means that the particles carried away from the gasifier by the product gases can be captured in an external cyclone and be circulated to the gasifier.

Pneumatic transport region is evolved from a fast fluidized-bed when the gas velocity keeps increasing. As shown in Figure 2, all particles are lifted up by the gas stream. A large scale migration of particles occurs due to higher gas velocity, and the distribution of particles becomes more uniform than circulating fluidized bed gasifiers.

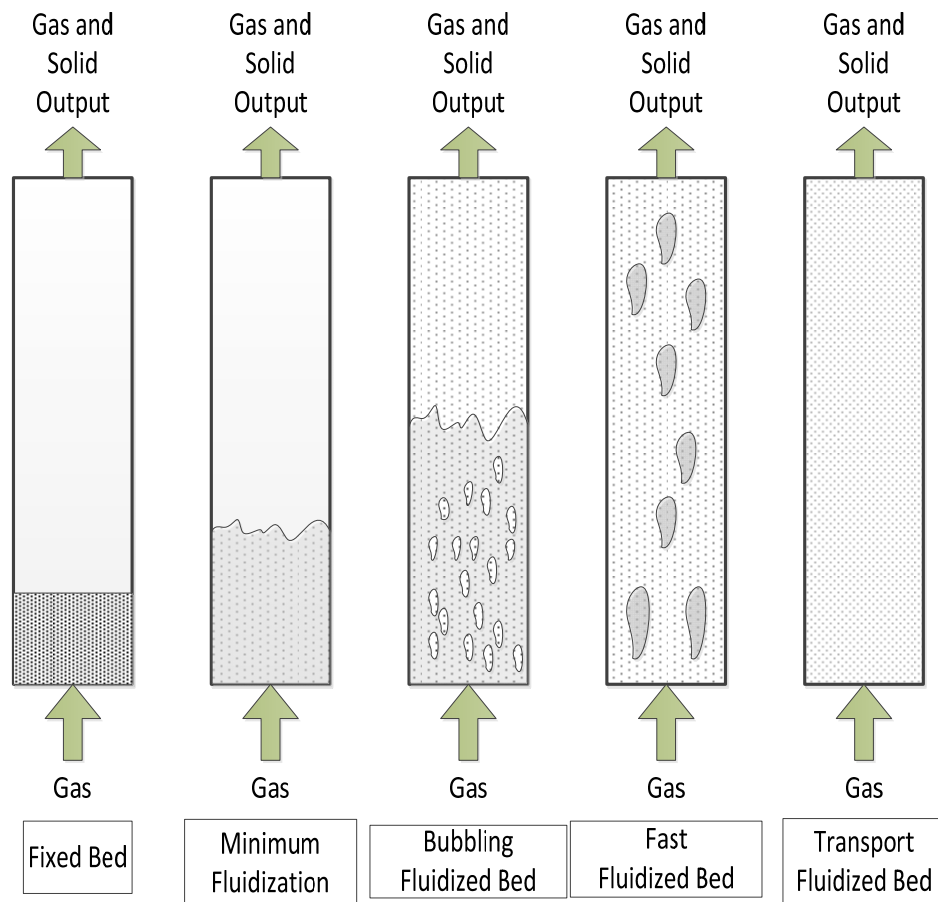


Figure 2: Transition from a Fixed Bed to a Transport Bed Gasifier

As another type of gasifier, entrained flow gasifiers are essentially concurrent reactors. In an entrained gasifier, pulverized coals, together with the gasifying mediums (oxygen and steam), are injected into the gasifier to generate syngas. Entrained flow gasifiers are widely applied in commercial gasification plants. However, this type of gasifier is mainly designed for coal gasification and may not be suitable for biomass gasification. In entrained gasifiers, coal is generally pulverized to tiny particles to gain high fuel conversion. However, biomass pulverization can be hardly implemented and the cost of biomass pulverization can be very high. On the other hand, biomass may be unable to provide the same amount of energy as a coal to maintain the high temperature operation of an entrained gasifier, given that the heating values of biomasses (about 17.5-20.8 MJ/kg for wood) are much lower than coals (about 36-37 MJ/kg for Anthracite [7]).

Therefore, compared with entrained gasifiers, fluidized bed gasifier such as BFB and CFB gasifiers are more favorable for biomass gasification. Among all types of fluidized gasifiers, the technology of CFB gasifier is more promising, considering the fact that in such a gasifier turbulent flow pattern provides better mixing between gases and biomass particles and more efficient heat and mass transfer.

However, due to the complexity of multiphase turbulent flows in circulating fluidized bed gasifiers, design and scale-up of such type of gasifiers becomes very challenging. Currently, the design of fluidized bed gasifier is mostly based on empirical correlations and experimental work. However, this issue can be addressed by more detailed CFD modeling, and the detailed patterns of velocity, gas composition, and temperature inside gasifiers can also be useful for gasifier design and process optimization.

1.2 Research Objectives and Scope

As shown in Figure 3, a comprehensive computational fluid dynamics (CFD) model, consisting of hydrodynamics, mass transfer and energy transfer modules, will be developed and utilized to simulate CFB biomass gasification using ANSYS Fluent software and C programming language.

In the hydrodynamics module, the Eulerian-Eulerian approach is applied to build this CFD model, the solid phase is treated as a continuum. According to the kinetic theory of granular flow, phase pressure, and bulk viscosity of the solid phase can be estimated by the fluctuation energy equation. The equation of motion is coupled with the standard k-epsilon turbulence model to simulate the hydrodynamics of gas-particle system in the CFB gasifier.

In the mass transfer and energy transfer modules, the species transport equation is applied to describe the gas composition distributions and the energy equation is used to simulate thermal conduction, convection, and radiation in the gasifier. The kinetics of heterogeneous char reactions and homogeneous gas phase reactions are integrated with the mass and energy conservation equations to simulate chemical reactions in the CFB gasifier.

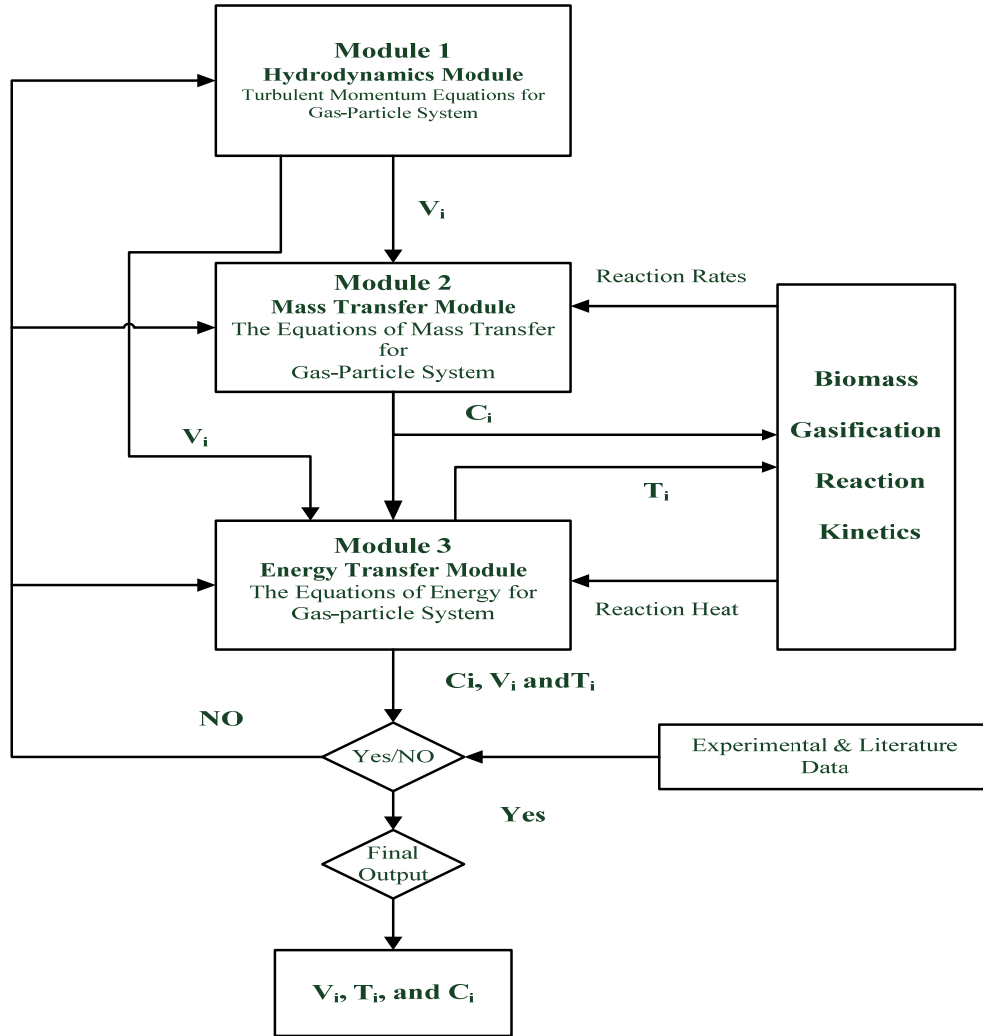


Figure 3: Simulation Framework of Biomass Gasification in a CFB

The main motive of this research is to build a framework of CFD modeling of biomass gasification using a CFB reactor, and the CFD model can be further used as a tool for design and process optimization of such type of gasifiers. In order to fulfill our goal, the following tasks will be done:

- To build a hydrodynamic model to describe the profiles of solid volume fraction and investigate the impact of drag model and standard wall function on the CFD modeling of gas-particle system in a riser of the CFB system.
- To establish a three dimensional (3D) steady-state CFD model to predict the profiles of velocity, solid volume fraction, temperature, and gas composition in a

CFB gasifier, and examine the effect of thermal radiation, the water gas shift reaction (WGS), and the equivalence ratio (ER), on the CFD modeling of CFB biomass gasification.

- To set up a three dimensional unsteady-state CFD model to investigate the effect of char combustion on the predictions of gas composition and gasifier temperature in a CFB biomass gasifier.

1.3 Thesis Outlines

Chapter 2 mainly describes hydrodynamic simulation of a gas-particle system in a riser. A literature review of hydrodynamic study is presented in Section 2.1. The descriptions of mathematical model are provided in Section 2.2. The settings of hydrodynamic model are described in section 2.3. In section 2.4, the simulation results are compared and validated by experimental data and the impacts of the standard wall function and drag models are also discussed. The conclusions of hydrodynamic model are presented in Section 2.5.

Chapter 3 mainly discusses the CFD modeling of CFB biomass gasification. A literature review of biomass gasification simulation is first given in the introduction section. The governing equations such as the momentum, mass, and energy equations as well as the kinetics of heterogeneous char reactions and homogeneous gas-phase reactions are provided in Section 3.2. The impact of thermal radiation, the water gas shift (WGS) reaction, and the equivalence ratio are discussed in the section of Results and Discussion.

Chapter 4 is mainly focused on the role of char combustion production distribution coefficient in the CFD modeling of biomass gasification. The mathematic model and the settings are presented in Section 4.2 and 4.3, respectively. The effect of distribution coefficient of char combustion on the predictions of gas composition and temperature is discussed in Section 4.4 and is summarized in Section 4.5.

Finally, the conclusions of the current studies and the recommendations for future work are summarized in Chapter 5.

Chapter 2

CFD Modeling of Gas-Particle Flow in a Circulating Fluidized Bed Riser*

2.1 Introduction

Circulating fluidized bed (CFB) is widely applied in many chemical processes, such as biomass gasification, combustion, and catalytic cracking [8, 9]. However, optimal design and scale-up of a CFB system is quite challenging due to the complexity of turbulent flow pattern in risers serving as reactors in the systems. Thus, a quantitative understanding of hydrodynamics of the gas-particle system in the risers is crucial for designing such systems [10].

The turbulent flow patterns of gas-particle system in the risers are generally simulated in two approaches: Eulerian-Lagrangian and Eulerian-Eulerian methods [11]. In the Eulerian-Lagrangian approach, the gas phase is regarded as a continuum, while the particle phase is treated as a discrete phase. Trajectories of particles as well as mass and momentum transfer are calculated using the soft sphere or hard sphere model. The simulation using this approach requires enormous amount of computing resources because every particle in the system is tracked and calculated at the same time. Thus, this approach may not be efficient for the simulation of a large-scale CFB, which generally contains millions of particles [12].

The Eulerian-Eulerian (E-E) approach consumes much less computing resources. In this technique, both gas and particle phases are considered as interpenetrating continuum. The conservation of mass and momentum equations are applied as governing equations, and the interphase momentum transfer is described by drag models [13]. Due to the assumption of continuum, the properties of solid phase such as phase pressure, shear viscosity, and bulk viscosity need to be defined explicitly. A fluctuating energy equation was then developed from the kinetic theory of granular flow and was applied to calculate these properties for the closure of governing equations [14, 15].

* Liu H., Biglari M., Elkamel A., Lohi A., The Impacts of Standard Wall Functions and Drag Model on the Turbulent Modeling of Gas-Particle Flow in a Circulating Fluidized Bed Riser. The Canadian Journal of Chemical Engineering, 91(2013)707-714.

Numerous works have been done for modeling of granular flow in risers of CFB, but many of them were laminar models [9, 16-19], as the kinetic theory of granular flow was initially developed and applied for laminar models [20].

The hydrodynamic models were mainly established and developed for the simulations of chemical processes such as fluid catalytic cracking, circulating fluidized bed gasification and combustion [13, 21]. To this purpose, the laminar “cold” models (hydrodynamic models) need to be further integrated with mass and energy transport equations. However, since the hydrodynamic systems in these processes are definitely turbulent, regarding the effects of heat and mass transfer in turbulent flows, turbulence models are more appropriate than laminar models. Thus, in this chapter, a turbulence model is established and integrated with the kinetic theory of granular flow to simulate the hydrodynamics of gas-particle system in a riser. The main focus of this study is to develop not only a purely hydrodynamics model but also a model potentially applicable for simulations of chemical processes.

For hydrodynamic studies, the profile of solid concentration in the near-wall region is an emphasis. For laminar models, the semi-empirical boundary equations proposed by Johnson and Jackson [22] were proved to be effective to predict the distribution of particles in the near-wall region [9], while, for turbulence models, the boundary conditions are generally controlled in the wall functions to simulate the dramatic change of momentum and energy. Because of the importance of boundary conditions, the impacts of wall function are investigated in this chapter.

Solid distributions in risers can also be significantly influenced by different types of drag models. The drag model developed by Gidaspow, et al. [23] is commonly used. However, as claimed by Yang, et al. [21], the conventional drag models may not be adequate methods for the heterogeneous flow structures in dense solid phases, because this type of drag model was mainly derived from the experimental data of homogenous systems.

Another type of drag model, the energy-minimization multi-scale (EMMS) approach, was reportedly capable of predicting the heterogeneous structure of dense solid phase [21, 24]. In this chapter, both of these two types of drag models were tested and compared.

Additionally, the impact of particle-particle restitution coefficient is also examined, as it plays an important role in simulating hydrodynamics of particle-gas system [15].

2.2 Gas-particle model description

2.2.1 Continuity equations

Mass balance for each phase is computed by the following continuity equations [25]:

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla \cdot (\alpha_g \rho_g \mathbf{v}_g) = 0 \quad (1)$$

$$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla \cdot (\alpha_s \rho_s \mathbf{v}_s) = 0 \quad (2)$$

where ρ and $\mathbf{v}$ are the density and velocity for each phase, respectively, α is the volume fraction, g and s stand for the gas phase and the particle phase, respectively.

2.2.2 Conservation of momentum equations

Due to turbulent flow patterns in risers of CFB, turbulent momentum equations are appropriate for modeling of the gas-particle hydrodynamics.

The Momentum equations for turbulent flow include:

$$\frac{\partial (\alpha_g \rho_g \mathbf{v}_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g \mathbf{v}_g \mathbf{v}_g) = -\alpha_g \nabla p + \nabla \cdot (\boldsymbol{\tau}_g + \boldsymbol{\tau}_g') + \alpha_g \rho_g \mathbf{g} + \beta (\mathbf{v}_s - \mathbf{v}_g) \quad (3)$$

$$\frac{\partial (\alpha_s \rho_s \mathbf{v}_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s \mathbf{v}_s \mathbf{v}_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \cdot (\boldsymbol{\tau}_s + \boldsymbol{\tau}_s') + \alpha_s \rho_s \mathbf{g} + \beta (\mathbf{v}_g - \mathbf{v}_s) \quad (4)$$

where p is the pressure, β is the drag coefficient, $\boldsymbol{\tau}_g$ and $\boldsymbol{\tau}_s$ are the laminar stress tensors for the gas and particle phases, respectively, and $\boldsymbol{\tau}_g'$ and $\boldsymbol{\tau}_s'$ are the Reynolds stress tensor for the gas and particle phases, respectively. They are defined as follows [26]:

$$\tau_{g,s} = \alpha_{g,s} \mu_{g,s} (\nabla \mathbf{v}_{g,s} + \nabla \mathbf{v}_{g,s}^T) + \alpha_{g,s} (\xi_{g,s} - \frac{2}{3} \mu_{g,s}) \delta \quad (5)$$

where μ is the shear viscosity, ξ is the bulk viscosity, and δ is an unit tensor. ξ_g is zero for a gas.

$$\tau_{g,s}' = \alpha_{g,s} \mu_{g,s}^t (\nabla \mathbf{v}_{g,s} + \nabla \mathbf{v}_{g,s}^T) - \frac{2}{3} (\alpha_{g,s} \rho_{g,s} k_{g,s} + \alpha_{g,s} \mu_{g,s}^t \nabla \cdot \mathbf{v}_{g,s}) \delta \quad (6)$$

and

$$\mu_{g,s}^t = \rho_{g,s} C_\mu \frac{k_{g,s}^2}{\varepsilon_{g,s}} \quad (7)$$

where μ^t is the turbulent viscosity, k is the turbulent kinetic energy, ε is the dissipation rate of turbulent kinetic energy, and $C_\mu = 0.09$ [27].

k and ε are modeled in the following modified k-epsilon equations for multiphase flow [27]:

$$\frac{\partial}{\partial t} (\alpha_i \rho_i k_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i k_i) = \nabla \cdot \left(\alpha_i \frac{\mu_i^t}{\sigma_k} \nabla k_i \right) + (\alpha_i G_{k,i} - \alpha_i \rho_i \varepsilon_i) + \beta (C_{ij} k_j - C_{ji} k_i) - \beta (\mathbf{v}_j - \mathbf{v}_i) \frac{\mu_j^t}{\alpha_j \sigma_j} \nabla \alpha_j + \beta (\mathbf{v}_j - \mathbf{v}_i) \frac{\mu_i^t}{\alpha_i \sigma_i} \nabla \alpha_i \quad (8)$$

$$\frac{\partial}{\partial t} (\alpha_i \rho_i \varepsilon_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i \varepsilon_i) = \nabla \cdot \left(\alpha_i \frac{\mu_i^t}{\sigma_\varepsilon} \nabla \varepsilon_i \right) + \frac{\varepsilon_i}{k_i} \left[C_{1\varepsilon} \alpha_i G_{k,i} - C_{2\varepsilon} \alpha_i \rho_i \varepsilon_i + C_{3\varepsilon} \left(\beta (C_{ji} k_j - C_{ij} k_i) - \beta (C_{ji} k_j - C_{ij} k_i) \frac{\mu_j^t}{\alpha_j \sigma_j} \nabla \alpha_j + \beta (\mathbf{v}_j - \mathbf{v}_i) \frac{\mu_i^t}{\alpha_i \sigma_i} \nabla \alpha_i \right) \right] \quad (9)$$

where i, j stand for the gas and particle phase, $i = g, s$, $j = s, g$; σ_k , σ_ε , $C_{1\varepsilon}$, $C_{2\varepsilon}$, and $C_{3\varepsilon}$ are 1.0, 1.3, 1.44, 1.92, and 1.2, respectively [28, 29]. Other parameters are defined as follows:

$$G_{k,i} = \mu_i^t S^2 \quad (10)$$

$$S = \sqrt{S_{ml}} \quad (11)$$

$$S_{ml} = \frac{1}{2} \left(\frac{\partial v_m}{\partial v_l} + \frac{\partial v_l}{\partial v_m} \right) \quad (12)$$

$$C_{ji} = 2, \text{ and } C_{ij} = 2 \left(\frac{\eta_{ji}}{1 + \eta_{ji}} \right) \quad (13)$$

where m, l represent coordinate directions, and η_{ji} is defined as:

$$\eta_{ji} = \frac{\tau_{ji}^t}{\tau_{ji}^F} \quad (14)$$

$$\tau_{ji}^t = \frac{\tau_i^t}{\sqrt{1 + C_\beta \zeta^2}} \quad (15)$$

$$\tau_{ji}^F = \frac{\alpha_j \rho_j}{\beta} \left(\frac{\rho_j}{\rho_i} + C_V \right) \quad (16)$$

$$\zeta = \frac{|v_{ji}| \tau_i^t}{L_i^t} \quad (17)$$

$$\tau_i^t = \frac{3}{2} C_\mu \frac{k_i}{\varepsilon_i} \quad (18)$$

$$L_i^t = \sqrt{\frac{3}{2}} C_\mu \frac{k_i^{\frac{3}{2}}}{\varepsilon_i} \quad (19)$$

$$C_\beta = 1.8 - 1.35 \cos^2 \theta \quad (20)$$

where $C_V = 0.5$, and θ is the angle between the average particle velocity and the relative velocity [27]. The k-epsilon equations are applied to both the gas and particle phases.

2.2.3 Fluctuating energy equation

The kinetic theory of granular flow was developed from classical kinetic theory of non-uniform dense gases, assuming the random motion of particles analogous to the thermal motion of gas molecules [30]. According to this theory, the pressure and viscosity of particle phase are closely related to the random motion of particles. A concept “granular temperature” was introduced, and it was defined to be proportional to the kinetic energy of particle motion [31]. An energy balance equation, so-called fluctuating energy equation, was formulated for the kinetic energy of particle random motion in which the energy was generated by the particle shear stress and was dissipated through the inelastic collisions between the particles [32]. Using Equations 21 to 25, the fluctuating energy equation (Eq. 26) is defined.

Particle phase pressure:

$$p_s = \alpha_s \rho_s \Theta [1 + 2(1+e)g_0\alpha_s] \quad (21)$$

where Θ is the granular temperature

Bulk viscosity of particle phase:

$$\xi_s = \frac{4}{3} \alpha_s \rho_s (1+e) \left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} \quad (22)$$

where e is the restitution coefficient.

Shear viscosity of particle phase:

$$\mu_s = \frac{2\mu_{dil}}{(1+e)g_0} \left[1 + \frac{4}{5}(1+e)g_0\alpha_s\right]^2 + \frac{4}{5} \alpha_s^2 \rho_s d_p g_0 (1+e) \left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} \quad (23)$$

$$\mu_{dil} = \frac{5\sqrt{\pi} \rho_s d_p \Theta^{\frac{1}{2}}}{96} \quad (24)$$

where d_p is the particle diameter, and g_0 is the radial distributional function and is defined as follows:

$$g_0 = \frac{3}{5} \left[1 - \left(\frac{\alpha_s}{\alpha_{smax}} \right)^{\frac{1}{2}} \right]^{-1} \quad (25)$$

where α_{smax} is the maximum volume fraction of the particle phase.

Fluctuating energy equation:

$$\frac{3}{2} \left[\frac{\partial \alpha_s \rho_s \Theta}{\partial t} + \nabla \cdot (\alpha_s \rho_s \Theta \mathbf{v}) \right] = (\tau_s) : \frac{\partial \mathbf{v}}{\partial \mathbf{r}} - \nabla \cdot \mathbf{q} - \gamma - 3\beta\Theta \quad (26)$$

where $\mathbf{q}$ is the flux of fluctuating energy and is defined as:

$$\mathbf{q} = -\kappa \nabla \Theta \quad (27)$$

$$\kappa = \frac{150\sqrt{\pi} \rho_s d_p \Theta^{\frac{1}{2}}}{384(1+e)g_0} \left[1 + \frac{6}{5}(1+e)g_0\alpha_s \right]^2 + 2\alpha_s^2 \rho_s d_p (1+e) \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} \quad (28)$$

and γ is the collisional energy dissipation rate, defined as follows:

$$\gamma = 3(1-e^2)\alpha_s^2 \rho_s g_0 \Theta \left(\frac{4}{d_p} \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} - \nabla \cdot \mathbf{v}_s \right) \quad (29)$$

In this simulation work, the default setting for modeling granular temperature in the software of Fluent is used by neglecting the convection and diffusion terms in Equation-26 [27].

2.2.4 Interphase momentum exchange between the gas and particle phases

The interphase momentum exchange has a major impact on momentum balance for each phase, and is described by the multiplication of the drag coefficient β to the slip velocity. There are many drag coefficient models, but they are mainly in two categories: the conventional drag models and the energy minimization multi-scale models (EMMS) [33].

2.2.4.1 Conventional drag models

The conventional drag models were generally derived from the data of particle terminal velocity and pressure drop, and the mostly applicable model was proposed by Gidaspow et al. (1992). This model is a combination of the Wen and Yu model [34] and the Ergun equation [35] in which the calculation of drag coefficient is switched between the two models using a porosity condition as shown below:

For $\alpha_g \leq 0.8$

$$\beta_{Ergun} = 150 \frac{\alpha_s^2 \mu_g}{\alpha_g d_p^2} + 1.75 \frac{\rho_g \alpha_s |v_g - v_s|}{d_p} \quad (\text{Ergun model}) \quad (30)$$

For $\alpha_g > 0.8$

$$\beta_{Wen\&Yu} = \frac{3}{4} C_d \frac{\rho_g \alpha_s \alpha_g |v_g - v_s| \alpha_g^{-2.65}}{d_p} \quad (\text{Wen and Yu model})$$

(31)

$$C_d = \frac{24}{\alpha_g Re_p} [1 + 0.15(\alpha_g Re_p)^{0.687}] \quad (32)$$

$$Re_p = \frac{\rho_g |v_g - v_s| d_p}{\mu_g} \quad (33)$$

Based on Gidaspow's model, an additional switch function and a correlation factor, φ , shown below, were formulated by Lu and Gidaspow [13] to attain a smooth transition between the two coefficient calculations.

$$\beta = \varphi \beta_{Ergun} + (1 - \varphi) \beta_{Wen\&Yu} \quad (34)$$

$$\varphi = \frac{\arctan[150 \times 1.75 (0.2 - \alpha_s)]}{\pi} + 0.5 \quad (35)$$

2.2.4.2 EMMS models

Some energy minimization multi-scale (EMMS) models were developed to describe heterogeneous nature of gas-solid fluidization and the model results were reported to gain a good agreement with experimental data.

In the EMMS approach, the flow in a riser is considered to consist of two pseudo phases, cluster and dilute phases [33]. The momentum equations were first applied to the dense phase, the dilute phase, and all of the particles, respectively. The pressure balance between the dense and dilute solid phase as well as the mass balance between the gas and particles were also established. Based on the constraints defined by the momentum and mass balance equations, an objective function to minimize the energy for suspending the whole solid phase was then solved [33]. The flow structure parameters such as diameter, fraction of clusters, and the slip velocity can be obtained through minimizing the energy under given conditions. All of these parameters will be used to compute a so-called “structure based” drag coefficient, which will be incorporated into a conventional drag model to calculate the interphase momentum exchange in a gas-particle system [36].

A drag correlation model using EMMS approach was derived by Yang, et al. [21] based on some simplifications on the calculations of parameters such as the voidage at minimum fluidization, the maximum voidage for particle aggregating, and the voidage of dense phase. This drag model is shown as follows [21]:

Yang model:

For $\alpha_g < 0.74$

$$\beta_{Ergun} = 150 \frac{\alpha_s^2 \mu_g}{\alpha_g d_p^2} + 1.75 \frac{\rho_g \alpha_s |v_g - v_s|}{d_p} \quad (\text{Ergun model}) \quad (36)$$

For $\alpha_g \geq 0.74$

$$\beta_{Wen\&Yu} = \frac{3}{4} C_d \frac{\rho_g \alpha_s \alpha_g |v_g - v_s|}{d_p} \omega \quad (37)$$

$$\omega = -0.5760 + \frac{0.0214}{4(\alpha_g - 0.7463)^2 + 0.0044} \quad \text{for } 0.74 \leq \alpha_g \leq 0.82 \quad (38)$$

$$\omega = -0.0101 + \frac{0.0038}{4(\alpha_g - 0.7789)^2 + 0.0040} \quad \text{for } 0.82 < \alpha_g \leq 0.97 \quad (39)$$

$$\omega = -31.8295 + 32.8295\alpha_g \quad \text{for } \alpha_g > 0.97 \quad (40)$$

2.2.5 Standard Wall conditions

Many experiments have found that three types of layers exist in the near-wall region for turbulent flows: the layer closest to the wall is called as “viscous sub-layer” in which the flow is mainly laminar and the laminar viscosity plays a dominant role; the outmost layer is the “inertial sub-layer” where the turbulent flow is fully developed; the layer between these two layers is named as buffer layer [37].

The flow conditions in the near-wall region are very important for modeling turbulent flows because the variations of velocity in this region are significant and have a big impact on the mean velocity of bulk flow [38].

The so-called “standard wall functions” are used to describe the velocity distribution in the near-wall region. For the computational fluid dynamics (CFD), instead of solving the velocities in each layer separately, the nodal velocities in the wall-adjacent cells are generally solved using only one set of equations, either the one for inertial sub-layer or viscous sub-layer as shown below [39]:

A dimensionless velocity U^* and a wall unit y^* were defined below:

$$U^* = \frac{U_p C_\mu^{\frac{1}{4}} k_p^{\frac{1}{2}}}{\tau_w / \rho} \quad (41)$$

$$y^* \equiv \frac{\rho C_\mu^{\frac{1}{4}} k_p^{\frac{1}{2}} y_p}{\mu} \quad (42)$$

where U_p is the mean velocity at the nodal point P of the wall-adjacent cell, and y_p is the distance between the point P and the wall.

Then, for $11.225 < y^* < 300$ (inertial sub-layer)

$$U^* = \frac{1}{\kappa} \ln(Ey^*) \quad (43)$$

and for $y^* < 11.225$ (viscous sub-layer)

$$U^* = y^* \quad (44)$$

where κ and E are a constant, 0.4187 and 9.793, respectively [27].

As indicated by Albets-Chico, et al. [38], the wall functions for the inertial sub-layer are more preferable and can provide more correct approximation for modeling of high Reynolds number flows than the functions for the viscous sub-layer.

2.3. Simulation parameters and settings of the particle-gas system

All of the equations were solved in Fluent using finite volume method. The simulation results for the particle-gas system were validated by the experimental data from Parssinen and Zhu [40] and Parssinen [41]. The simulations were implemented on the 2-D grids, which were discretized non-uniformly in the radial direction and were divided equally in the axis direction. The computational grids have the identical dimensions with the experimental risers. However, since the experimental data is only available for a half of riser, considering axisymmetric structure of the riser, a half of the computational geometry was built with a radial distance of 0 to $D/2$ for this simulation work.

The particle velocity at the inlet was specified as a constant and was calculated by the following equations:

$$v_{s,inlet} = \frac{G_s}{\rho_s \alpha_{s,inlet}} \quad (45)$$

where G_s is the solid mass flux, and $\alpha_{s,inlet}$ is the solid volume fraction at the inlet.

The gas velocity at the inlet was specified by the following parabolic profile:

$$v_{g,inlet} = \frac{2v_{g,up}}{(1-\alpha_{s,inlet})} \left[1 - \left(\frac{r}{R} \right)^2 \right] \quad (46)$$

where $\alpha_{s,inlet}$ is the solid volume fraction at the inlet, $v_{g,up}$ is the gas superficial velocity, r is the radial distance from the riser's centerline to the measuring point, and R is the radius of the riser. The pressure at the outlet was set as a constant, atmospheric pressure. The wall functions were applied to both of the gas and particle phases.

The coupling and correction between pressure and velocity were solved using the SIMPLE algorithm [42]. For the 2-D unsteady-state model, the size of time step was 0.001 second with 500 iterations to achieve fully convergence at every time step. The profile of volume fraction was time-averaged after reaching the quasi-steady state. The convergence criterion of 1×10^{-3} was selected for the absolute scaled residual between two sequential iterations. The detailed modeling settings of the particle ($67 \mu m$)-gas system were shown in Table 1.

Table 1: Flow properties and simulation parameters of the particle ($67\mu m$)-gas system

Properties of gas and particle flows	Parameter values
Mean Particle diameter (d_p)	$67 \mu m$
Density (ρ_s)	$1500 kg/m^3$
Solid mass flux (G_s)	$300 kg/m^2 s$
Superficial gas velocity ($v_{g,sup.}$)	$5.5 m/s$
Boundary conditions	
Inlet condition (gas, particle)	Velocity inlet
Volume fraction of particle phase at	0.25
Outlet condition (gas, particle)	Atmospheric pressure
Wall condition (particle)	No-slip
Wall condition (gas)	No-slip
Computational Grid Settings	
Inner diameter of the riser (D)	$76 mm$
Height of the riser	$10 m$
Radial distance from the centerline (r)	$38 mm$
Number of cells	15×400
Modeling methods and settings	
Multiphase modeling approach	Eulerian-Eulerian
Turbulent flow modeling	k-epsilon equations
Gas-solid drag model	Gidaspow's model
Restitution coefficient	0
Granular temperature modeling	Algebraic

2.4 Simulation results and discussions of the particle-gas system

2.4.1 Grid study for the standard wall functions

In this section, four grids with different resolutions 4000-cell grid (10×400), 6000-cell grid (15×400), 8000-cell grid (20×400), and 12000-cell grid (30×400), are built, and the

volume fraction profiles at various heights are compared with the experimental data [40, 41]. The schematic diagram of 6000-cell grid is shown in Figure 4.

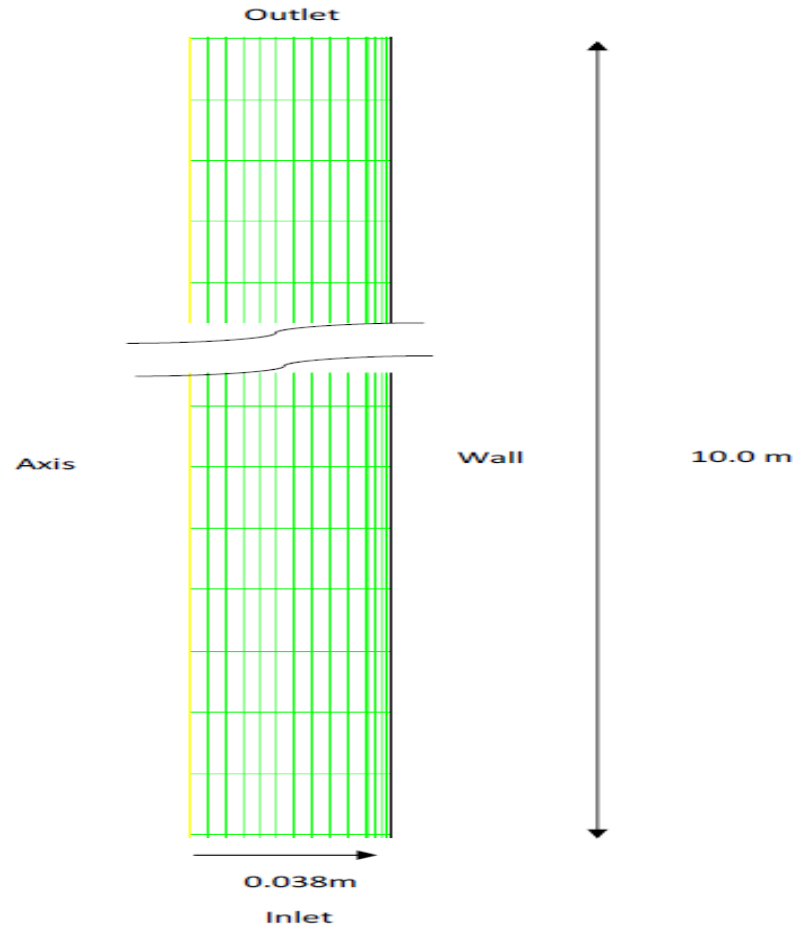


Figure 4: Schematic Diagram of 6000-cell (15x400) Grid

All of the simulations from the three grids, 4000-cell grid, 6000-cell grid, and 8000-cell grid, predict a core-annular flow structure, a main feature of solid flows in risers where dense solids mainly accumulate in the near-wall region while dilute solids move upwards in the core of the riser [43].

The comparisons between the predicted profiles of solid volume fraction and the experimental data at the heights of 6.34 and 9.42 meters are shown in Figures 5 to 8. Figures 5 and 6 show that the volume fraction profile from the 6000-cell grid presents a better prediction than the 4000-cell grid. As shown in Figures 7 and 8, the most matched

simulation results are still from the 6000-cell grid, the 8000-cell grid provides very similar results, and the worst predictions are from the 12000-cell grid.

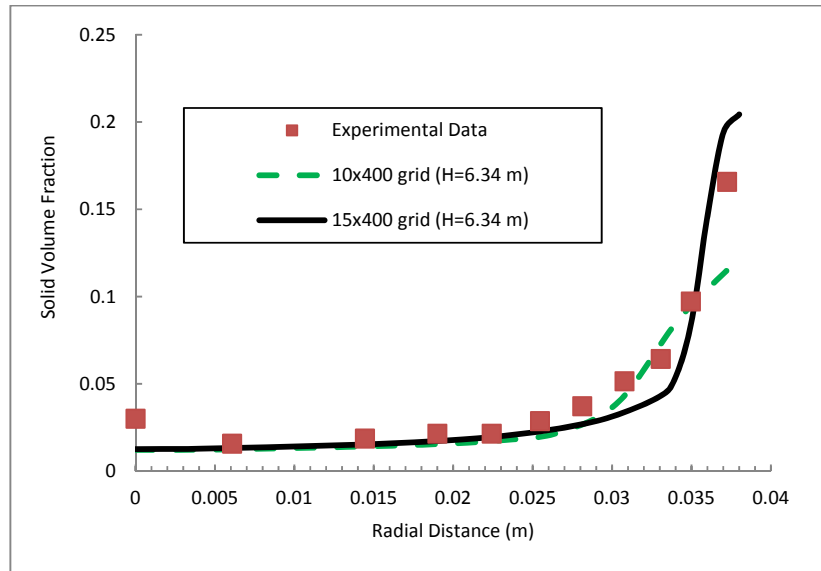


Figure 5: Comparison of Solid Volume Fraction: 4000-cell Grid vs. 6000-cell Grid (H=6.34)

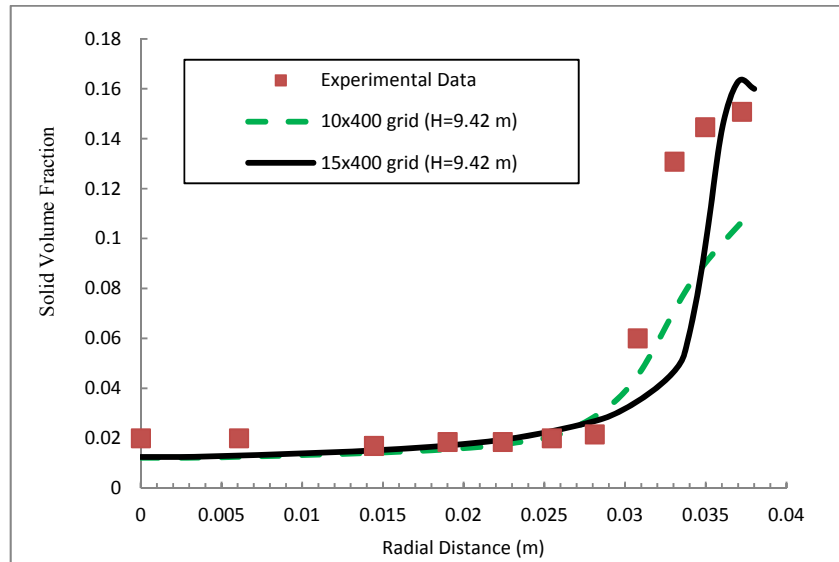


Figure 6: Comparison of Solid Volume Fraction: 4000-cell Grid vs. 6000-cell Grid (H=9.42)

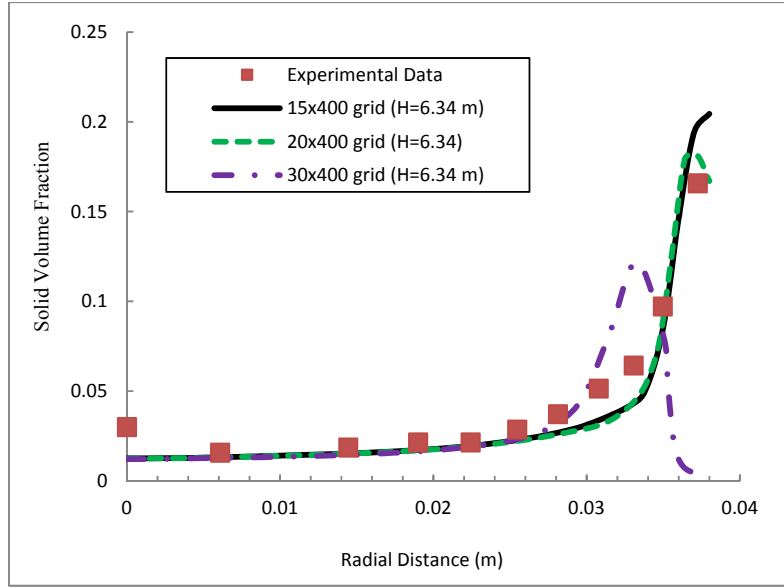


Figure 7: Comparison of Solid Volume Fraction: 6000-cell Grid vs. 8000-cell Grid vs. 12000-cell Grid ($H=6.34$)

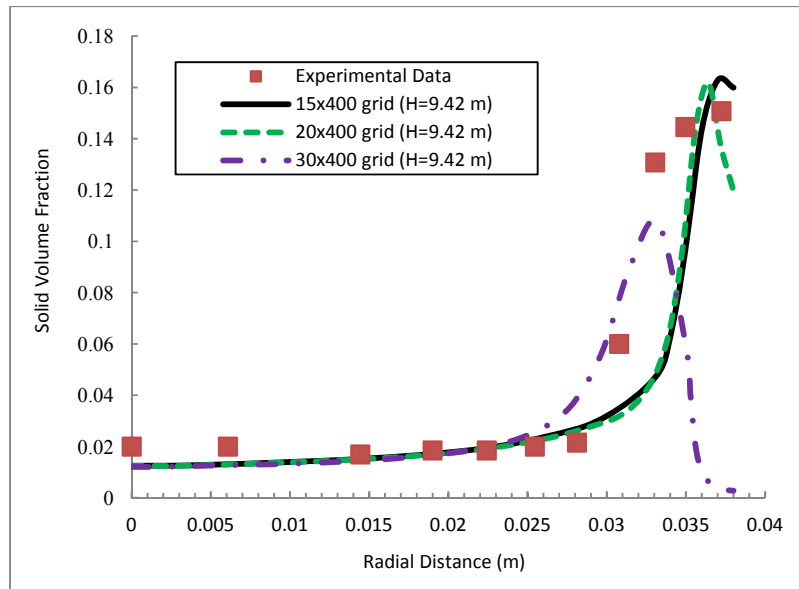


Figure 8: Comparison of Solid Volume Fraction: 6000-cell Grid vs. 8000-cell Grid vs. 12000-cell Grid ($H=9.42$)

It is seen that the excessively fine grid (12000-cell) does not provide a good prediction for the turbulence model. It seems that the principle of grid independence is not followed in the near-wall region. As indicated by Fluent [27], the simulation results for turbulent flows may tend to be grid-dependent, compared with laminar flows, and the similar

trends of grid-dependence in the near-wall region were also observed by Salim and Cheah [44].

The standard wall functions were actually derived from a set of “semi-empirical” formulae, in which the law-of-the-wall or the logarithmic law of the wall was assumingly followed for the momentum and temperature in the near-wall region [27, 37]. Saving computation resources is the main reason that the wall functions are widely applied in CFD software. On the other hand, in case that a fully numerical approach is used, since the transport properties in the near-wall region generally change very quickly i.e., hundreds of times faster than the rest of fluid, very fine meshes in the near-wall region are then required for a good accuracy. The computation time for this region can reach up to 3-300 times of computation time required for the rest of fluid; meanwhile, the part of this region only accounts for 1% of the fluid volume [45].

In spite of the simplicity of the wall functions, the grid-dependence in the near-wall region appears to be an issue for the applications of the functions [46]. Considering that the logarithmic law of the wall is only effective in the inertial sub-layer ($11.225 < y^+ < 300$, defined in Fluent), one should follow the main premise for the standard wall functions strictly: the grid point in the first cell near the wall needs to be placed in the fully turbulent inner region (for this study, also called as inertial sub-layer) [47]. A very close or faraway location for the first grid node may result in worse predictions for the near-wall region [46, 48]. Noticing that the accuracy of standard wall function depends on the values of y^+ of the near-wall mesh, Chieng and Launder B.E. [49], Johnson and Launder [50], and Craft, et al. [51] made some efforts to improve the formulae. However, since this type of model is still in the process of being improved and developed, the complete grid independence in the near-wall region may not be guaranteed.

In this case study, the wall functions coupled with the turbulence model are separated in two sets of equations: the wall functions for the inertial sub-layer and the ones for the viscous sub-layer. The selection of the set of functions will depend on the range of y^+ ,

which is proportional to y_p , the distance between the cell centroid P and the wall, shown in Equation 42.

Since the values of y_p for the 12000-cell grid are smaller than the 6000-cell grid, the values of y^* for the 12000-cell grid are also smaller than the ones of the 6000-cell grid, as shown in Figure 9. Therefore, the wall functions for the viscous sub-layer are then applied to the 12000-cell grid; in other words, the computation boundary layer of 12000-cell grid is narrower than the actual inertial sub-layer of turbulent flows and falls in the region of actual viscous sub-layer. As the standard wall function may not present very accurate results for the viscous sub-layer, a discrepancy from simulation results is then observed.

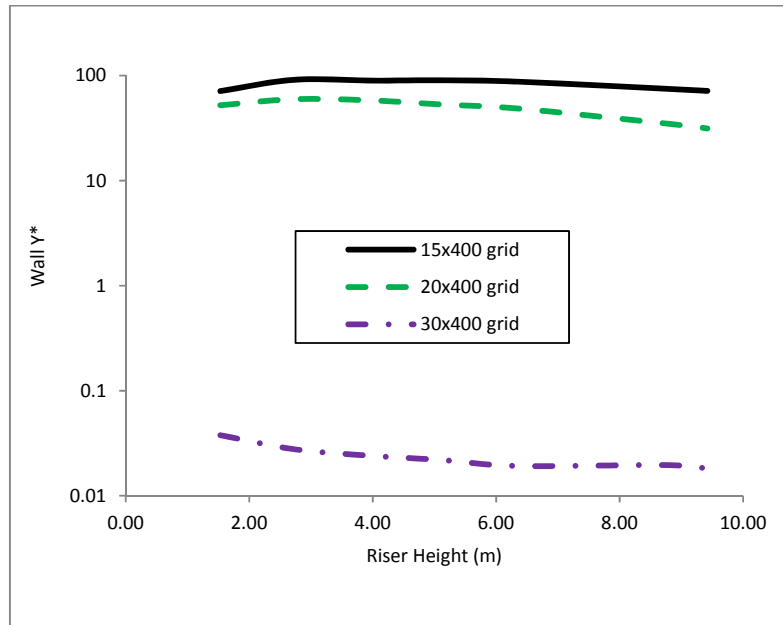


Figure 9: Comparison of Y^* Value: 6000-cell grid vs. 8000-cell grid vs. 12000-cell grid
However, as seen in Figures 5 to 8, in most of the regions of computation geometry except the near-wall region, the principle of grid independence is still well-followed in the radial range of 0-0.03 m. All of the four grids from the coarse grid to the finest one, the predictions are very similar and gain a good agreement with the experimental data.

It is found that the wall functions play a significant role in the near-wall region for the turbulence model and a mesh with proper value of y^* ($11.225 < y^* < 300$) is desirable for the turbulence model. In this case study, both the coarse grid (4000-cell) and the excessively fine grid (12000-cell) does not provide a good prediction due to the grid dependence of the stand wall functions.

2.4.2 Particle- particle restitution coefficient

The particle-particle restitution coefficient, in the range of 0 to 1.0, is another influential factor, which can affect particle phase pressure, solid bulk, and shear viscosities based on the kinetic theory of granular flow. Restitution coefficient of 1.0 indicates the particle collisions are elastic, whilst the coefficient of less than 1.0 means that the particle collisions are inelastic.

As shown in Figures 10 and 11, case 1 (restitution coefficient =0) presents a better prediction than case 2 (restitution coefficient=1.0). The main reason is that a higher value of restitution coefficient may generate a higher prediction of solid viscosity, as shown in Figure 12. This relationship between restitution coefficient and solid viscosity was also found by Cloete and Amini [15].

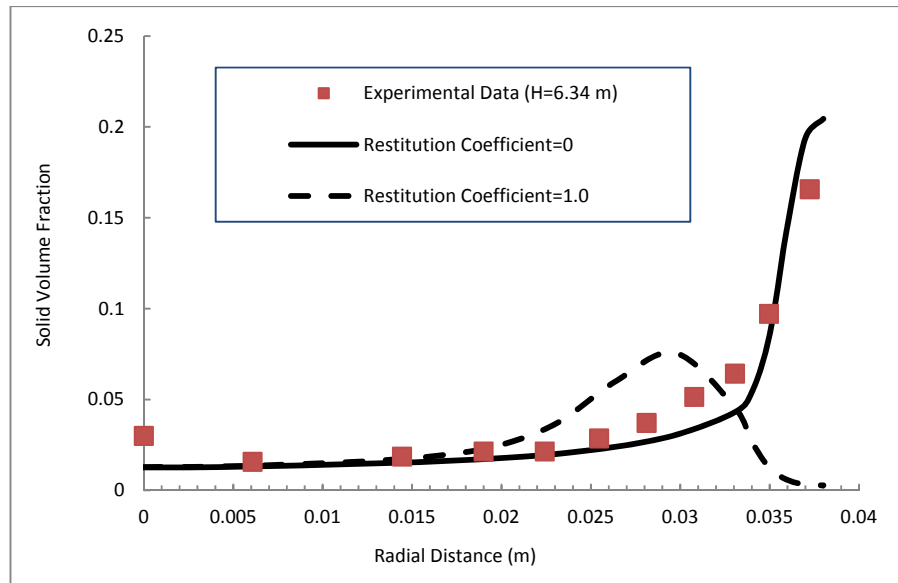


Figure 10: Solid Volume Fraction Profiles using Different Restitution Coefficients: $e=0$ vs. $e=1.0$ ($H=6.34$ m)

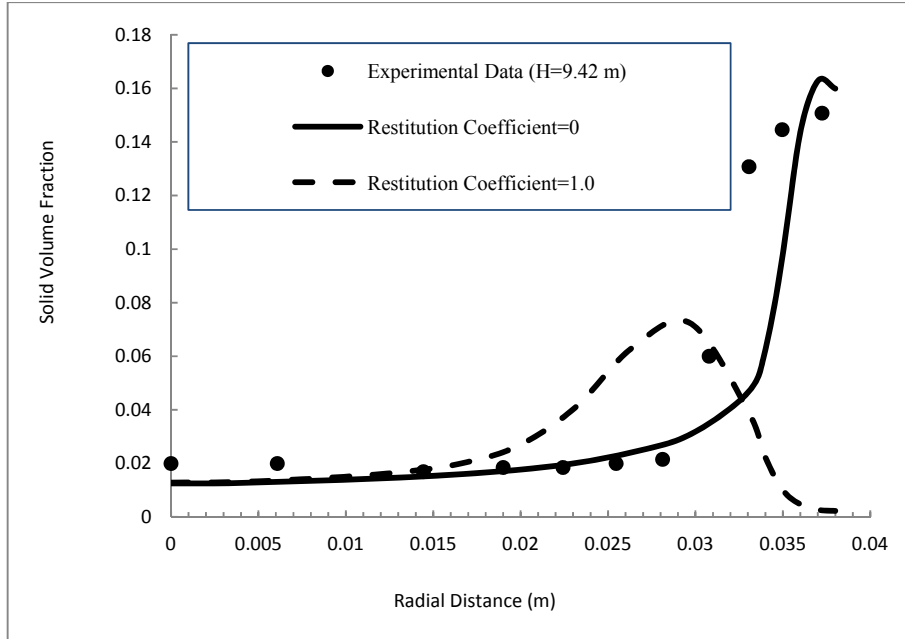


Figure 11: Solid Volume Fraction Profiles using Different Restitution Coefficients: $e=0$ vs. $e=1.0$ ($H=9.42$ m)

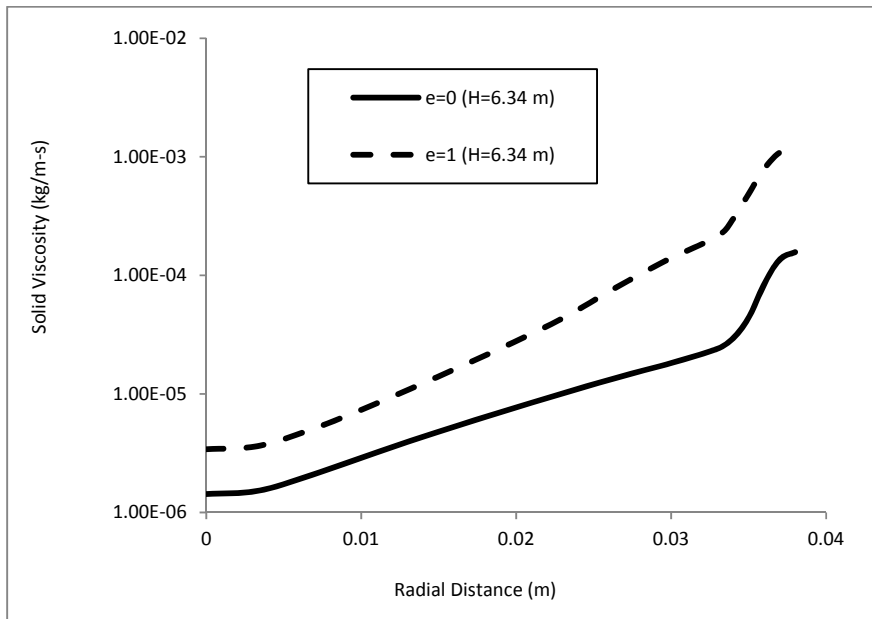


Figure 12: Solid Viscosity Comparison: $e=0$ vs. $e=1.0$

According to Equation 42, the value of viscosity is inversely proportional to the value of wall y^* , the value of y^* in case 2 is then much smaller than the one of case 1, as illustrated in Figure 13. Again, the role of standard wall function starts to take effect, and

the functions of inertial sub-layer, highly recommended for turbulent flow, are then applied to case 1, while the functions of viscous sub-layer are used for case 2. So, similar to the grid study, the discrepancies are then observed in case 2.

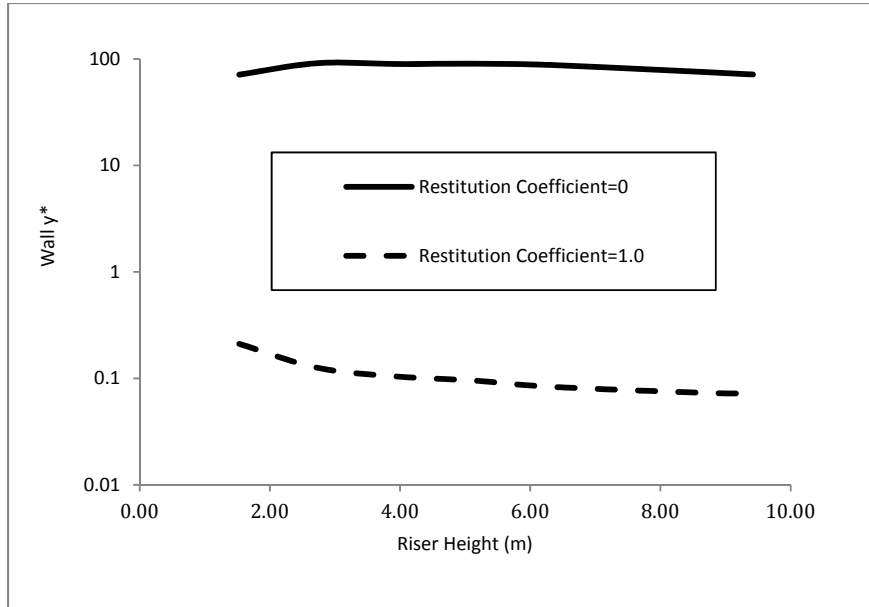


Figure 13: Comparison of Wall y^* : $e=0$ vs. $e=1.0$

As discussed above, the impact of restitution coefficient is important. The restitution coefficient, as an important tuning parameter, must be applied in caution [15]. The impact of standard wall functions can't be neglected for turbulence models when the value of restitution coefficient is changed. Varying the value of restitution coefficient may influence the predictions of solid viscosity and the values of wall y^* , and consequently, the discrepancies of solid fraction profiles may be generated due to the grid dependence of standard wall functions. It should be noted that the role of restitution coefficient for turbulence model may be different from the one for laminar models, as the standard wall functions are only coupled with turbulence models. Therefore, for laminar models, the impact of restitution coefficient on the prediction in the near-wall region may not be as obvious as this study.

2.4.3 Conventional drag coefficients vs. EMMS drag coefficients

Interphase momentum exchange, described by drag coefficient, plays an important role in the momentum balance of the gas-particle system. As mentioned earlier, there are

numerous drag models for granular flows, which are mainly categorized into two types of models, the conventional and the EMMS models. In this study, three drag models, Gidaspow's, Lu's, and Yang's models, are individually coupled with the turbulence model to investigate the impacts on the predictions of solid volume fraction in the riser.

As mentioned by Yang, et al. [21], flow structures in risers are actually heterogeneous rather than homogeneous, and the formations of clusters are evident when the particles act with the air. As shown in Figure 14, a cluster-based structure is seen in the contour plot of solid fraction from Yang's model. In Figure 15, a temporal-varying feature is also shown in the profile of the averaged volume fraction from Yang's model, and each peak point indicates a passing of particle cluster. The similar temporal-varying characteristic was seen from the experimental data of Zhu and Zhu [52] and the simulation results of Atsonios, et al. [24]. In comparison with the EMMS models, as indicated by our simulation, the averaged solid volume fraction from Gidaspow's model is mostly constant after the quasi-steady state. The patterns of solid distribution in the riser are mainly uniform as displayed in Figure 16. The temporal-varying feature and cluster-based structure are not seen from the profiles of Gidaspow's Model. It may be because the conventional models were mainly developed from the homogeneous experimental data such as the data from fixed beds [21].

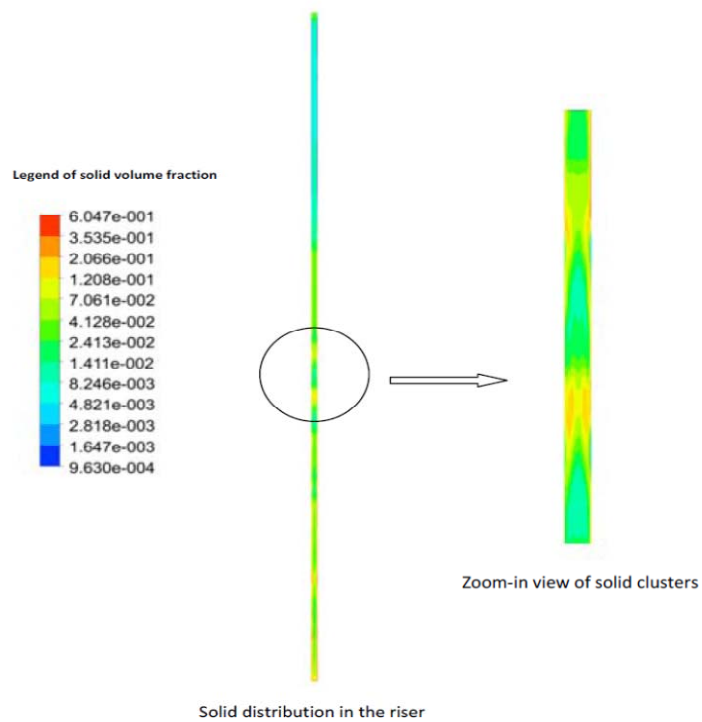


Figure 14: Contour of Solid Volume Fraction from Yang's (EMMS) Model

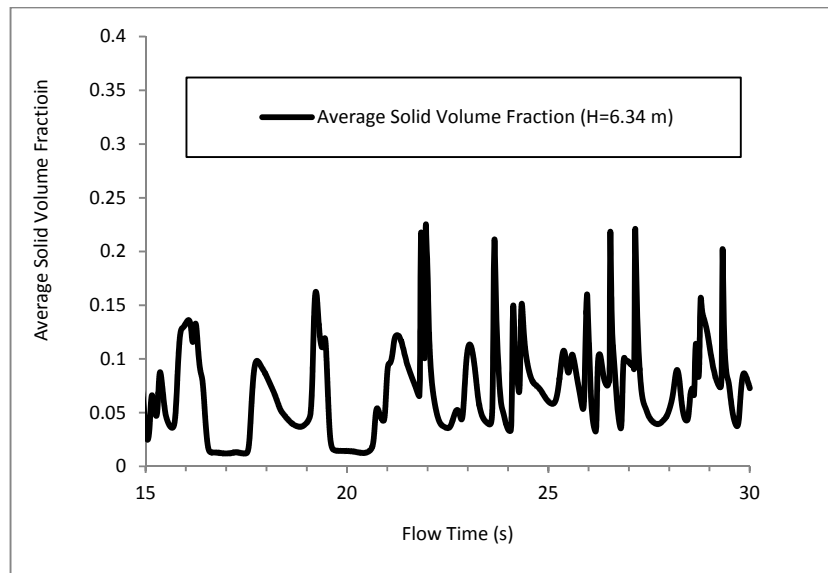


Figure 15: Time-series of Volume Fraction Profile at H=6.34 meter (EMMS Model)

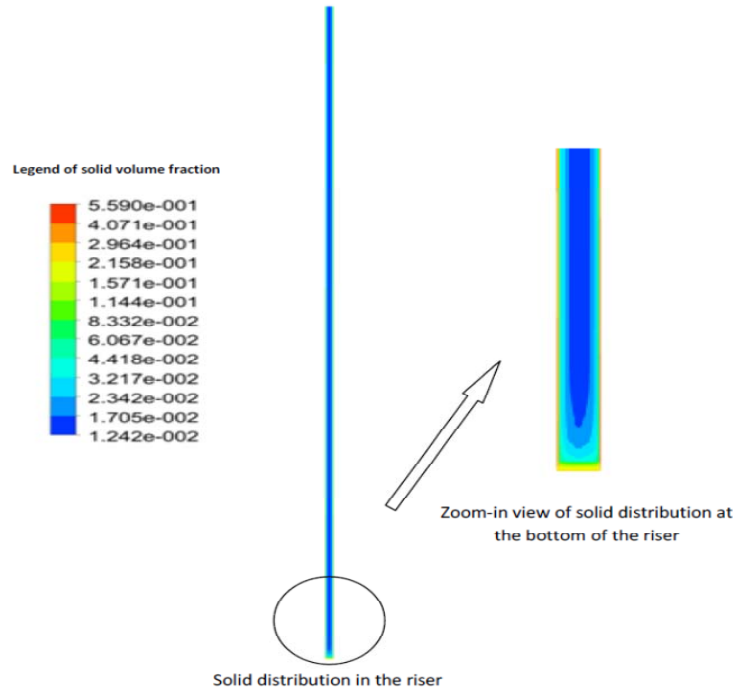


Figure 16: Contour of Solid Volume Fraction from Gidaspow's Model

In Figure 17, it is clearly seen that the profile from Yang's model demonstrates three regions existing in the riser: dense-phase region with high solid concentration at the bottom of the riser, transition-phase region with intermediate solid concentration in the middle of the riser, and dilute-phase region with low solid concentration at the top of the riser, which follow the similar trend as indicated by Zhu and Zhu [52], whilst in the profile from Gidasopow's model, the transition from dense to dilute phase is not as obvious as the former. However, it should be noted that in the bottom part of the riser, the averaged solid volume fraction from both of the two models are smaller than the experimental data. The underestimation of solid volume fraction by CFD models was also observed by other researchers [9, 16, 53]. The discrepancy may be due to the simplifications of computation for dealing with such complex systems [9].

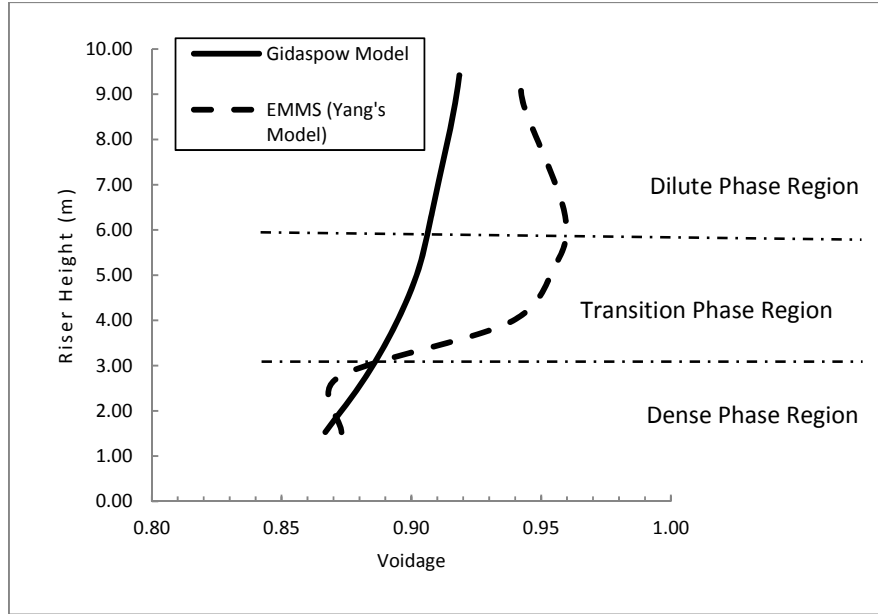


Figure 17: Comparison of Axial Voidage Profiles: Gidaspow Model vs. EMMS Model

As shown in Figures 18 and 19, the profile of Lu's model is quite similar to Gidaspow's model, and in Figure 19, these two profiles fully overlap. It is also shown that EMMS model (Yang's model) doesn't present a good agreement with the experimental data in the radial direction. It may be because the EMMS models were mainly developed under some specific settings of flow structures such as cluster diameter corrections, the voidage of minimum fluidization, and the voidages of pseudo dilute and dense phases[21, 33]. These settings may be effective for the system described by Yang, et al. [21], but they may not be fully suitable for the current flow system. As mentioned by Shah, et al. [33], an EMMS model based on one particular flow system may not be fully valid in another flow system, and this may cause the discrepancies as seen in Figures 18 and 19.

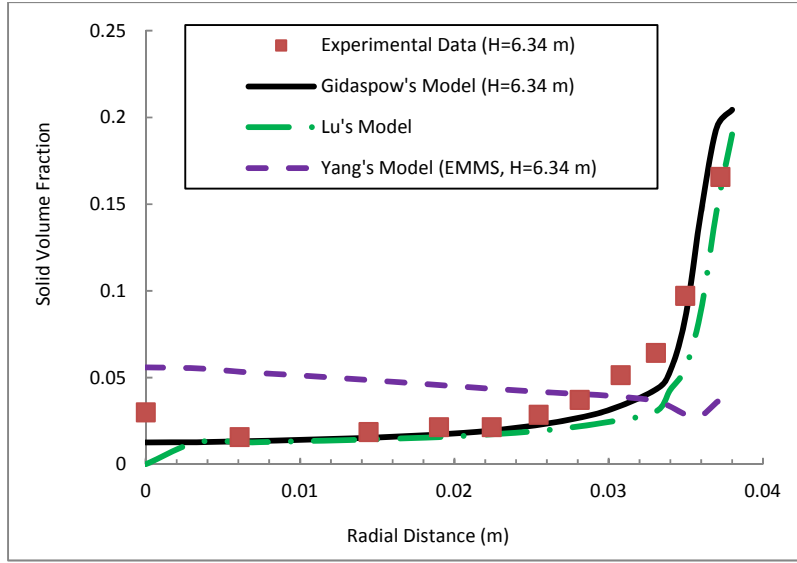


Figure 18: Comparison of Solid Volume Fraction Profiles: Conventional Models vs. EMMS Model at H=6.34 m

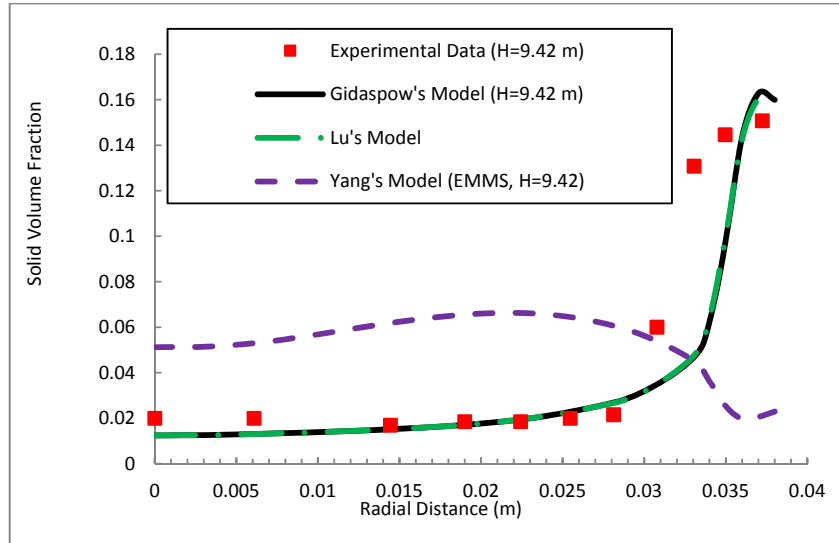


Figure 19: Comparison of Solid Volume Fraction Profiles: Conventional Models vs. EMMS Model at H=9.42 m

However, as seen in Figures 14, 15, and 17, Yang's model or the EMMS models can at least capture three main features of solid flow such as cluster formations, temporal varying profile, and three distinct solid phases in a riser. Should the appropriate structure parameters be available for this gas-particle system in the future study, the discrepancy can definitely be improved.

2.5 Conclusions

A 2-D gas-solid multiphase model incorporated with the kinetic theory of granular flow was built to simulate the granular flow in a riser for a small particle ($67\ \mu\text{m}$)-gas system, and the k-epsilon turbulent equations were applied to simulate turbulent behaviors in the fluidized bed riser. The simulation results were compared with the experimental data of Parssinen and Zhu [40] and Parssinen [41], and a good agreement was achieved.

A grid study was conducted to examine the impact of grid discretization on the simulation results. From the comparisons, it was seen that the role of wall functions was significant for turbulence models, and in this study the functions of inertial sub-layer were preferable for this particle-gas system, and the 6000-cell grid with proper values of y^* ($11.225 < y^* < 300$) present a good prediction.

Different types of drag models were integrated with the turbulent model and the simulation results were compared with the experimental data [40, 41]. The comparisons showed that the prediction from the EMMS model could present a temporal-varying profile, and the profile was capable of demonstrating three distinct solid phases existing in a riser. On the other hand, a great discrepancy was found in the radial profile of solid volume fraction, but it may be improved by obtaining suitable parameter settings of EMMS model for the current flow situations.

The impact of restitution coefficient of particle to particle was also investigated for the turbulence model by varying the value of the coefficient. It was found that the effect of restitution coefficient for turbulence models was significant and adjusting restitution coefficient must be implemented cautiously.

Chapter 3

Computational Fluid Dynamics Modeling of Biomass Gasification in Circulating Fluidized-Bed Reactor using Eulerian-Eulerian Approach*

3.1 Introduction

Bioenergy is the energy stored in plants through photosynthesis. The energy can be released from biomass by thermal conversion processes such as combustion and gasification. Biomass gasification is an attractive technology. Gasification not only generates heat, but it also produces important intermediate chemicals such as syngas ($\text{CO} + \text{H}_2$), which is widely used in chemical industries [54]. Additionally, the conversion efficiency of gasification, which can reach up to 50%, is higher than the efficiency of combustion, about 20-40% [55].

Many types of biomass gasifiers are used in industry. Among these technologies, the gasification using circulating fluidized bed (CFB) has become more promising due to excellent mixing effects and efficient heat transfer in gasifiers [56]. Since the interactions of fluid mechanics and thermal conversion of biomass are very complicated, designing such type of gasifier is very challenging and is mainly based on empirical corrections derived from experiments in bench-scale or pilot plants. However, these empirical formulas can be only applied under certain conditions and do not have a very general application [57].

In recent years, remarkable progress has been achieved in improving the accuracy and stability of numerical techniques and algorithms. Computational fluid dynamics (CFD) has been applied as an important design tool in various industrial areas, and the CFD techniques have shown the ability to provide accurate prediction for some chemical processes [58]. Currently, for CFD simulations of coal or biomass gasification, there are mainly two types of methods, the Eulerian-Lagrangian approach, and the Eulerian-Eulerian approach.

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In the Eulerian-Lagrangian approach, the gas phase is described by the Navier-Stokes equations, while the solid phase is treated as a discrete phase. The trajectory of each particle is calculated by Newton's Laws of motion, and the collisions between particles are described by the model of soft-sphere or hard-sphere [59]. Other variables such as temperature and gas concentration are computed by the equations of energy and mass transfer for each particle. Since each particle in the system is tracked, the accuracy of simulation result may be improved, but meanwhile this approach also requires an enormous amount of computational resources. It might not be feasible for the simulations of large scale fluidized bed systems that generally contain millions of particles [60].

Compared with the Eulerian-Lagrangian approach, the Eulerian-Eulerian approach requires less amount of computation because the solid phase is treated as a continuum. In this approach, the transport properties of solid phase are estimated by the kinetic theory of granular flow [61].

The Eulerian-Eulerian approach was first used for the simulations of hydrodynamics of gas-particle systems in risers, and numerous models were developed [9, 16, 20], but they were called "cold" models and no chemical reactions were considered. With the development of computer hardware and the progress of numerical techniques and algorithms, the Eulerian-Eulerian approach has been recently applied to simulate coal and biomass gasification. Yu, et al. [62] presented a two-dimensional (2D) model of coal gasification in a bubbling fluidized bed, and Gerber et al. [60] proposed a similar model for wood gasification using bubbling fluidized bed. Li, et al. [63] built a 3D model of coal gasification in a pressurized spout-fluid bed gasifier, and Wang, et al. [64] developed a 3D model of coal gasification in a fluidized bed.

However, the previous works are mostly about coal gasification in a bubbling fluidized-bed, and very few works have been devoted to simulating biomass gasification in a circulating fluidized-bed (CFB). Considering abundant biomass resources in nature and the advantages of this technology, building a detailed model for CFB biomass gasification then becomes very necessary. The predicted patterns of momentum, mass, and energy transport in the gasifier can be valuable for the design and optimization of

gasifier. Therefore, the purpose of this work is to build a comprehensive model of CFB biomass gasification.

In some CFD models mentioned above, the state variables were computed in two dimensions, but 2D models may be inappropriate and insufficient for the modeling of gasification in fluidized beds. Since the structures of gasifiers using fluidized-beds are generally non-axisymmetric, the hydrodynamics of the gasifier can't be properly described by 2D axisymmetric models [63, 64]. Consequently, based on the improper prediction of flow pattern, the predictions for other variables such as gas composition and reactor temperature may also be inaccurate. In this chapter, the CFD model is solved in three dimensions and it will present more sufficient and accurate predictions than 2D models.

CFD models are generally solved on discretized grids by the numerical methods such as the finite difference, finite element, and finite volume methods. The error of simulation result generated from a coarse mesh can be significant, and it is very necessary to evaluate the effect of grid selection on the final solution [65]. However, the grid-independence study, which is to ensure the final solution independent of the mesh resolution, is rarely found in the previous works. In this chapter, a grid study is implemented to reduce the discretization error from the numerical method (finite control volume method), and accordingly the accuracy of the model will also be improved.

Additionally, based on some assumptions, the effect of thermal radiation on heat transfer in the gasifiers was claimed to be negligible in the previous Eulerian-Eulerian models [62-64, 66]. However, thermal radiation, as a major method of heat transfer, is important for gasification, and ignoring the effect of thermal radiation may compromise the accuracy of the model. For this work, the impact of thermal radiation is investigated to clarify the issue, and in order to describe heat transfer more thoroughly and accurately, all of the three types of heat transfer including thermal conduction, convection, and radiation are considered in the model.

Finally, the water-gas shift (WGS) reaction is a chemical reaction widely used in gasification models [66-68]. However, since the reaction kinetics were mostly obtained in

experiments with catalysts [69-71], considering the non-catalytic environment and short residence time in fluidized-bed gasifiers, the application of WGS reaction in the simulation of gasification may not be appropriate [72-75]. In this chapter, the WGS reaction is not included in the CFD model, due to its catalytic kinetics. Accordingly, the error from the modeling of reaction kinetics may also be minimized. The ability of the CFD model in accurately predicting results is also further tested in various cases by varying the equivalence ratio (ER).

3.2 Descriptions of Mathematical Model

In this chapter, a comprehensive 3D CFD model using the Eulerian-Eulerian approach is developed to simulate biomass gasification in a CFB reactor. The standard k-epsilon turbulence model is coupled with the kinetic theory of granular flow to simulate the hydrodynamics of gas-particle system in the gasifier. The equations of continuity, motion, and energy are integrated with the radiation mode (P-1) and reaction kinetics to compute mass and energy transfer in the system. The simulation results will be compared and validated with the experimental data from García-Ibañez, et al. [76].

Since the main focus of this work is to discuss the stable trends of gas composition and temperatures in the gasifier, for the sake of simplicity, the steady-state model is then applied to simulate the whole process, as proposed by Deng et al.[68]. So, all of the terms involving $\frac{\partial}{\partial t}$ in the following equations are zero. However, it should be noted that due to turbulent flows in gasifiers, flow patterns inside gasifiers are in a pseudo-steady state instead of an absolute steady-state. This model is therefore applied to describe the trends of transport properties.

3.2.1 Continuity Equation

The mass conservation equation for the solid and gas phases are:

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla \cdot (\alpha_g \rho_g v_g) = m_{gs} \quad (47)$$

$$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla \cdot (\alpha_s \rho_s v_s) = m_{sg} \quad (48)$$

where m_{gs} and m_{sg} are the source terms of mass generation or consumption for the gas and solid phases due to the heterogeneous reactions.

3.2.2 Equation of Motion and Standard k-epsilon Turbulence Model

The momentum equation is coupled with the standard k-epsilon turbulence model to simulate the hydrodynamics in the gasifier [77].

3.2.2.1 Equation of Motion and Standard k-epsilon Turbulence model

The equations of motion for the gas and solid phases are:

$$\frac{\partial(\alpha_g \rho_g v_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g v_g v_g) = -\alpha_g \nabla p + \nabla \cdot (\tau_g + \tau_g^t) + \alpha_g \rho_g g + m_{gs} v_s + \beta(v_s - v_g) \quad (49)$$

$$\frac{\partial(\alpha_s \rho_s v_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s v_s v_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \cdot (\tau_s + \tau_s^t) + \alpha_s \rho_s g + m_{sg} v_g + \beta(v_g - v_s) \quad (50)$$

where the gas and solid viscous stress tensor, τ , and Reynolds stress tensor, τ^t , are defined in Equations 5-7, and β is defined in Equations 30-33 by the Gidaspow model [23], as described in Chapter 2.

As depicted in Chapter 2, the standard k-epsilon turbulence model is defined in Equations 8-28, and is applied to both of the gas and solid phases.

3.2.2.2 Kinetic Theory of Granular Flow

In the Eulerian-Eulerian approach, the solid phase is treated as a continuum, and the transport properties of solid phase such as the shear viscosity and the bulk viscosity of the solid phase are modeled by the kinetic theory of granular flow [27, 61], which was described in Equations 21-29.

3.2.3 Equation of Energy

The energy transport equations for the gas and solid phases are:

$$\frac{\partial \alpha_g \rho_g E_g}{\partial t} + \nabla \cdot (\alpha_g \rho_g v_g E_g) = \nabla \cdot k_{eff,g} \nabla T_g + S_g + Q_{sg} \quad (51)$$

$$\frac{\partial \alpha_s \rho_s E_s}{\partial t} + \nabla \cdot (\alpha_s \rho_s v_s E_s) = \nabla \cdot k_{eff,s} \nabla T_s + S_s + Q_{gs} \quad (52)$$

where E is the specific enthalpy, k_{eff} is the effective thermal conductivity, T is the temperature, S is the source term of enthalpy change due to chemical reactions and thermal radiation, Q_{sg} and Q_{gs} are the intensity of heat exchange between the gas and solid phases, and $Q_{sg} = -Q_{gs}$.

The effective thermal conductivity is calculated by:

$$k_{eff} = k + \frac{C_p \mu^t}{Pr^t} \quad (53)$$

where k is the thermal conductivity, C_p is the heat capacity, and the value of the turbulent Prandtl, Pr^t , is set as 0.85.

3.2.3.1 Interphase Heat Transfer

The rate of heat transfer between the gas and solid phases is defined as follows [78]:

$$Q_{sg} = h_{sg}(T_s - T_g) \quad (54)$$

$$h_{sg} = \frac{6k\alpha_g\alpha_s Nu_s}{d_p^2} \quad (55)$$

$$Nu_s = (7 - 10\alpha_s + 5\alpha_s^2) \left(1 + 0.7Re_s^{0.2}Pr_s^{\frac{1}{3}}\right) + (1.33 - 2.4\alpha_s + 1.2\alpha_s^2)Re_s^{0.7}Pr_s^{\frac{1}{3}} \quad (56)$$

where h_{sg} is the heat transfer coefficient between the gas and solid phases, and Nu is the Nusselt number.

3.2.3.2 P-1 Radiation Model

As a method of heat transfer, thermal radiation is important for some chemical processes at high temperatures such as gasification and combustion. In this work, the P-1 model is applied to investigate the effect of thermal radiation in the gasifier. The P-1 model is a simplified form of P-N model and is defined as follows [27, 79]:

$$q_r = -\Gamma \nabla G \quad (57)$$

$$\Gamma = \frac{1}{3(a+\sigma_s)-C\sigma_s} \quad (58)$$

$$\nabla \cdot (\Gamma \nabla G) - aG + 4an^2\sigma T^4 = 0 \quad (59)$$

where q_r is the heat flux of thermal radiation, G is the incident radiation, a and σ_s are the absorption and scattering coefficients, respectively, C is the linear-anisotropic phase function coefficient, n represents the refractive index of the medium, and σ stands for the Stefan-Boltzmann constant.

The term, $-\nabla \cdot q_r$, is used to calculate the heat source due to thermal radiation in the equation of energy.

3.2.4 Species Transport Equations

The chemical species in the gasifier are computed by the species transport equations as follows:

$$\frac{\partial(\rho_g \alpha_g Y_{i,g})}{\partial t} + \nabla \cdot (\rho_g \alpha_g v_g Y_{i,g}) = -\nabla \cdot \alpha_g J_{i,g} + \alpha_g R_{i,g} + R \quad (60)$$

$$J_{i,g} = -\left(\rho_g D_{i,g} + \frac{\mu^t}{Sc_t}\right) \nabla Y_{i,g} - D_{T,i} \frac{\nabla T}{T} \quad (61)$$

where Y_i stands for the mass fraction of species i , J_i is the diffusion flux of species i , R_i is the net production rate of species i due to the homogeneous reactions, R is the net production rate of species i due to the heterogeneous reactions, D_i is the mass diffusion coefficient of species i , $D_{T,i}$ is the thermal diffusion coefficient of species i , and Sc_t is the turbulent Schmidt number.

3.2.5 Biomass Gasification Models

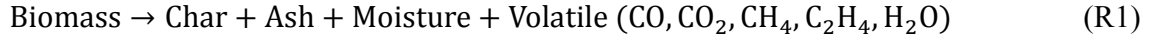
The chemical reactions in this model include the following processes: pyrolysis of biomass, heterogeneous reactions, and homogeneous reactions.

3.2.5.1 Pyrolysis of Biomass

Biomass pyrolysis is a thermochemical conversion process of biomass in the absence of air or oxygen. During the pyrolysis, the volatiles or tar are first released from biomass

particles to generate a mixture of gases; meanwhile biomass particles are transformed to carbonaceous solid particles in which the major element is carbon, known as “char”. Some pyrolysis models including single-step, two-step, and multi-step mechanisms were developed to describe the process [80].

Among these models, the two-step and multi-step schemes are usually used to describe both biomass devolatilization and tar cracking [80, 81]. In this chapter, due to lack of the data of tar in the literature [76], a single-step global scheme is applied instead to model biomass pyrolysis, but the two or multi steps can be considered for our future work in case the detailed modeling of devolatilization is required. The single-step global reaction for biomass pyrolysis is defined as follows:



In this study, the mass fractions of gas mixture released from the volatiles are determined from the proximate and ultimate analysis of biomass samples [62-64, 68].

The reaction rate is described by the Arrhenius equation:

$$r_p = k_p C_{bio} \quad (62)$$

$$k_p = f A T^n \exp \left(-\frac{E_a}{RT} \right) \quad (63)$$

where r_p is the reaction rate of biomass pyrolysis, k_p is the rate constant, C_{bio} is the concentration of un-reacted biomass particles, R is the universal gas constant, f is the fitting factor for pyrolysis reaction, and n is the exponent of the reaction temperature; A , the pre-exponent factor, and E_a , the activation energy, are set as 99.0 s^{-1} and 11.14 kJ/mol [82], respectively.

There is a wide variety of biomass in nature. The properties of biomass may vary significantly from one to another, and the kinetic data from different biomass samples may change accordingly. Hence, the kinetic data obtained from the samples of Yu et al.[82] may not be suitable for the one of biomass samples [76] used to validate the simulation model, and then using f and n to adjust the reaction rates may become necessary [60, 83]. In this work, the values of these two factors are set as 1510 and -1.2,

respectively. However, should the kinetic data for the biomass sample [76] be available in the future, they will definitely be used to improve the accuracy of our model.

3.2.5.2 Heterogeneous Reactions

In this work, the heterogeneous char reactions are:



A global reaction scheme that considers both the reaction kinetics and the diffusion rate is applied to the heterogeneous reactions [60, 62, 64, 67]:

$$r_{heter,i} = \frac{6V\alpha_s}{d_p} \cdot \frac{P_i}{\left(\frac{1}{k_{diff,i}} + \frac{1}{k_{kinet,i}}\right)} \quad (64)$$

$$k_{diff,i} = \frac{D_i Sh}{RT d_p} \quad (65)$$

$$D_i(T, P) = D(T_0, P_0) \left(\frac{T}{T_0}\right)^{1.75} \left(\frac{P_0}{P}\right) \quad (66)$$

$$Sh = 2 + 0.6Re^{\frac{1}{2}}Sc^{\frac{1}{3}} \quad (67)$$

$$k_{kinet,i} = A_i w_c^{-1} \exp\left(-\frac{E_i}{RT}\right) \quad (68)$$

where V is the volume of char particles, P_i is the partial pressure of gas species i , T_0 and P_0 are the reference temperature and pressure, respectively, k_{diff} is the mass transfer coefficient, k_{kinet} is the kinetic rate constant, Sh is the Sherwood number, and w_c is the molecular weight of char.

3.2.5.3 Homogeneous Reactions

The following homogeneous reactions are included in this study:



As discussed earlier, the roles of the water gas shift reaction, Equation-R10, are unclear because the reaction kinetics was obtained from the catalytic reactions [69-71]. In this chapter, Equation R10 is not used in the base case, but the effect of this reaction will be discussed in Section 3.4.5.

The rate constants of homogeneous reactions are modeled by the Arrhenius equations. The kinetic data of heterogeneous and homogeneous reactions are listed in Tables 2 and 3.

Table 2: Kinetic Data of Heterogeneous Reactions [84, 85]

Reaction No.	$A \left(\frac{\text{kg}}{\text{m}^2 \text{s Pa}} \right)$	$\frac{E}{R} \text{ (K)}$
R2	1.0×10^{-3}	3000
R3	6.35×10^{-3}	19500
R4	2.0×10^{-2}	8240
R5	1.18×10^{-5}	17921

Table 3: Kinetic Data of Homogeneous Reactions [86, 87]

Reaction No.	Reaction Rate Equations ($\frac{kmol}{m^3}$)	
R6	$r_6 = A_6 \exp(-\frac{E_6}{RT}) [CO][O_2]^{0.25} [H_2O]^{0.5}$	
R7	$r_7 = A_7 \exp(-\frac{E_7}{RT}) [H_2][O_2]$	
R8	$r_8 = A_8 T^{-1} \exp(-\frac{E_8}{RT}) [CH_4][O_2]$	
R9	$r_9 = A_9 \exp(-\frac{E_9}{RT}) [C_2H_4][O_2]$	
R10	$r_{10} = A_{10} \exp(-\frac{E_{10}}{RT}) \left([CO][H_2O] - \frac{[CO_2][H_2]}{K_{eq}} \right); K_{eq} = 0.0265 \exp(\frac{3968}{T})$	
Reaction No.	A	E ($\frac{kJ}{mol}$)
R6	$2.32 \times 10^{12} (kmol/m^3)^{-0.75} s^{-1}$	167
R7	$1.08 \times 10^{13} (kmol/m^3)^{-1} s^{-1}$	125
R8	$5.16 \times 10^{13} (kmol/m^3)^{-1} s^{-1} K$	130
R9	$1.0 \times 10^{12} (kmol/m^3)^{-1} s^{-1}$	173
R10	$12.6 (kmol/m^3)^{-1} s^{-1}$	2.78

3.3 Model Setup

In this chapter, a 3D steady-state model for the base case is built in accordance with the settings of the experiment[76], and the simulation results are also compared with the experimental data. The sizes of the gasifier are the same as the settings of the experiment: the inner diameter and the height of the gasifier are 0.2 and 6.5 meters, respectively. The properties of biomass samples and the operating conditions are listed in Tables 4 and 5.

Table 4: The Characteristic of Biomass sample [76]

Proximate Analysis (dry basis, wt %)	
Volatile Matter	74.4
Fixed Carbon	17.1
Ash	8.5
Ultimate Analysis (dry ash free basis, wt %)	
C	52.7
H	7.2
N	1.6
S	0.07
Cl	0.37
O	38.1
Lower Heating Values	18.5 MJ/kg

Table 5: Operating Conditions [76] and CFD model Settings

Operating Conditions	
Air Flow Rate (Nm ³ /h)	109
Biomass Feed Rate (kg/h)	60
Equivalence Ratio	0.41
Pressure (atm)	1.0
Boundary Conditions	
Air Inlet Condition	Velocity Inlet
Solid Inlet Condition	Mass Flow Inlet
Outlet	Pressure Outlet
Wall Conditions for the Gas and Particle phases	No-slip
CFD Model Settings	
Diameter of Computation Geometry	0.2 (meter)
Height of Computation Geometry	6.5 (meter)
Number of Computation Cell	366,249
Multiphase Modeling Approach	Euler-Euler
Drag Model	Gidspow's Model
Turbulence model	Standard k-epsilon Turbulence Model
Near Wall Treatment	Enhanced Wall Treatment
Radiation Model	P-1 model

The computation geometry and mesh are shown in Figures 20 and 21. The structured grid that consists of 366,249 cells is built for the gasifier. The CFD model is established and computed in Fluent 14.0. The flow rates of air and biomass solid are specified at the air and solid inlets, respectively, and the pressure at the outlet is set as the atmospheric pressure.

The finite volume method is applied to solve the governing equations. The least squares cell based method is utilized to calculate the gradients of the variables, and the algorithm of phase coupled SIMPLE is used to couple the pressure with the momentum equation and solve the set of discretized equations. The convergence criterion, scaled residual, is set as 2.0×10^{-5} for all of the transport equations.

Besides the base case study, other case studies are also established to study grid independence and investigate the impacts of turbulence models, radiation mode, and water shift reaction. Each of the simulations is computed in 200,000 iterations to ensure a converged and steady solution. The “wall clock time” for each case is approximately 7 days using a high performance computing cluster of twelve Intel X5670 cores at 2.9 GHz.

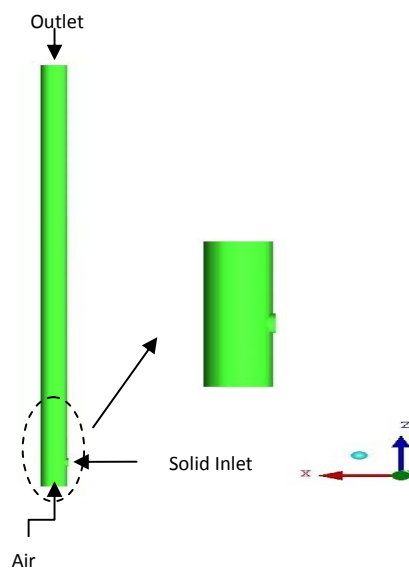


Figure 20: Computational Geometry of Gasifier

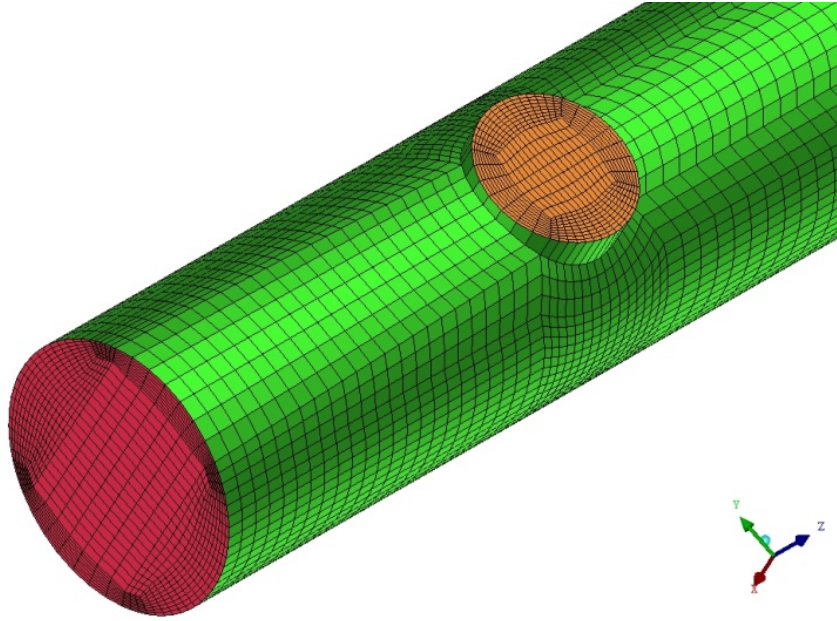


Figure 21: Structured Grid of Gasifier

3.4 Results and Discussion

In the base case study, the equations of continuity, motion, and energy integrated with the standard k-epsilon turbulence model and the P-1 radiation model are applied to simulate biomass gasification in a CFB reactor, using a grid with the resolution of 366,249 cells.

3.4.1 Results of Base Case

Figure 22 demonstrates the distribution of solid volume fraction at various heights in the gasifier. A typical core-annulus structure, the dilute suspension of solid in the center region and the dense suspension of solid in the near-wall region, is displayed in the figure. As shown in Figure 23, in the region adjacent to the wall, the solid velocity is close to zero due to the wall effect, while in the center region of the gasifier the solid velocity reaches a peak point. The similar trends of solid volume fraction and velocity bed in CFB reactors can also be seen in our other paper [77] and the reports by other researchers.[18, 88, 89].

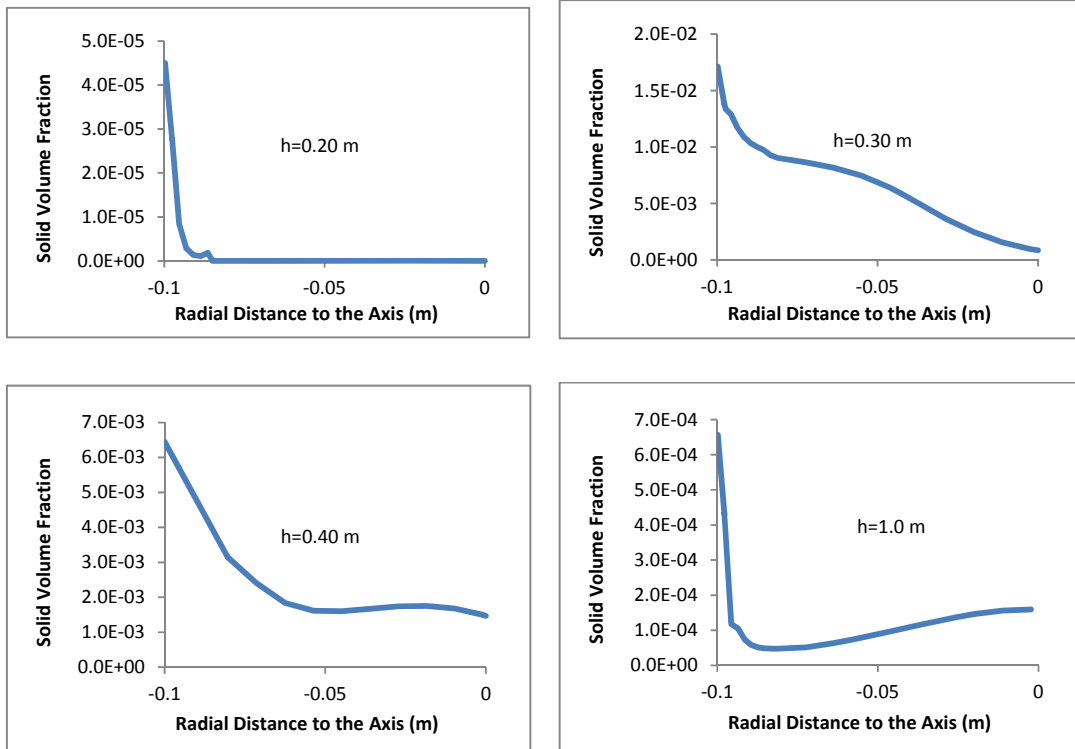


Figure 22: Solid Volume Fraction Profile

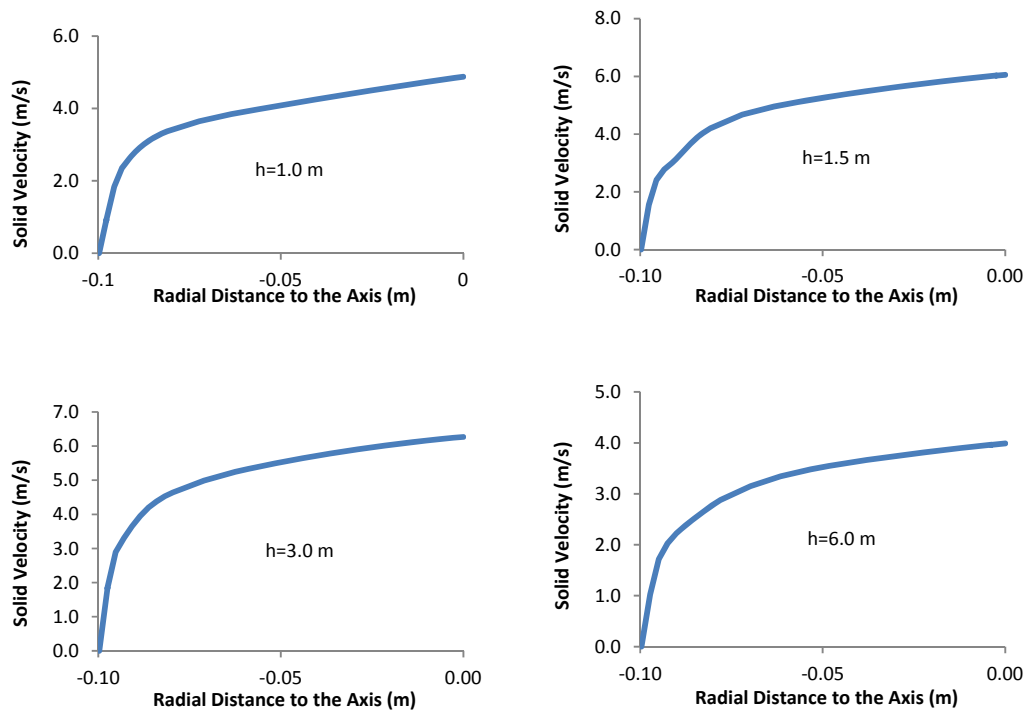


Figure 23: Velocity Profile of Solid Phase

The distributions of gas compositions in the gasifier are displayed in Figure 24. It can be seen that in the bottom area of the gasifier, CO, CO₂, CH₄, and C₂H₄ are generated from the volatiles during the pyrolysis. Char is also produced from the pyrolysis (reaction R1), and then it starts to react with H₂O to generate H₂ and CO (reaction R4). Due to the existence of O₂, the gas species are partly consumed by the combustion reactions in the middle part of the gasifier. Consequently, the mole fractions of CH₄ and C₂H₄ decrease until the combustion is finished. The mole fraction of CO does not drop as CH₄ and C₂H₄, due to the fact that CO can be generated not only from the pyrolysis but also from the reaction of char and H₂O (R4). The mole fraction of CO₂ increases constantly in the gasifier until O₂ is depleted due to the combustions of CO, CH₄, and C₂H₄.

Similar to CO, a decrease in the mole fraction of H₂ is hardly observed, and the mole fraction of H₂ keeps on increasing along the height of the gasifier. It may be because the combustible gases including CO, CH₄, and C₂H₄ are generated from the pyrolysis before H₂ is produced from reaction R4. Accordingly, most of O₂ may be already consumed by the volatile combustions, and there might be only a small amount of O₂ remained for the combustion of H₂. Meanwhile, H₂ is continuously generated from Reaction R4, and therefore a stable increase in the mole fraction of H₂ is seen in the axial direction of the gasifier. The similar trends of gas compositions in the gasifier can also be found in the report by Petersen and Werther [90].

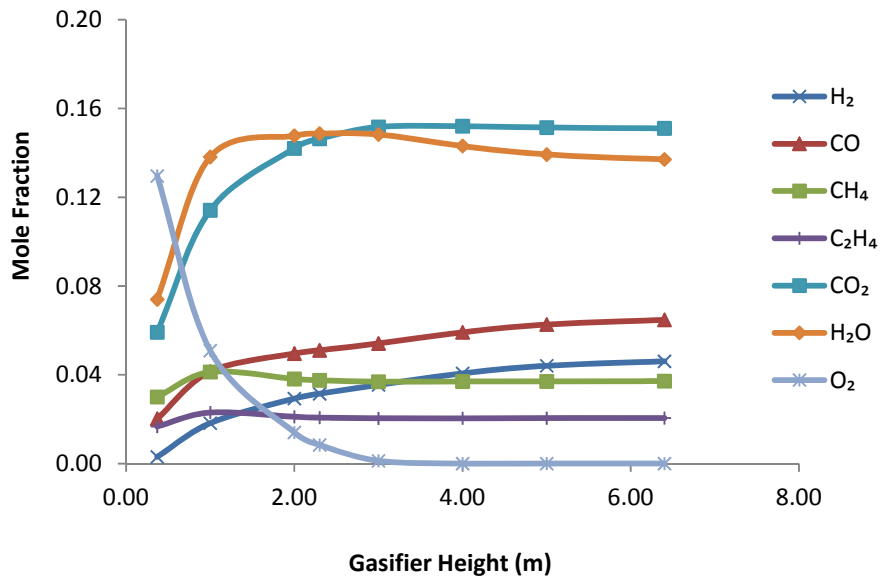


Figure 24: Mole Fraction Distribution of Gas Species in the Gasifier

The simulation results are also validated with the experimental data [76]. The outlet composition of CO, H₂, CH₄, C₂H₄, and N₂ are displayed in Figure 25 and are compared with the data. As seen in the figure, the differences are insignificant and the predicted gas compositions are in a good agreement with the measured values.

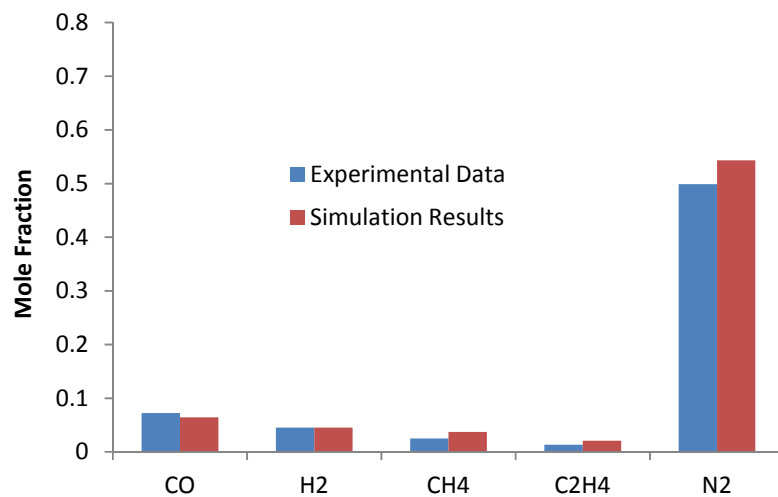


Figure 25: Predicted Outlet Gas Composition vs. Experimental Data

In order to further validate the CFD model, the predicted gasifier temperature profile is also demonstrated in Figure 26. As shown in the figure, the model predicts accurately two zones existing in the gasifier, the bottom region for pyrolysis and combustion between 0-2.3 meters, and the middle and upper regions for gasification between 2.3-6.5 meters, exactly as depicted in the literature [76]. In the zone of pyrolysis and combustion, the gasifier temperature increases quickly and reaches a peak due to the release of a large amount of combustion heat. In the zone of gasification, the temperature drops gradually along the height of the gasifier while the gasification reactions absorb the heat.

However, it can also be seen that the predicted peak temperature, approximately 1000 °C, is higher than the measured temperature from the experiment [76], around 800-900 °C. The overpredicted temperature profile is probably caused by the assumption of the Eulerian-Eulerian Approach that the particle phase is treated as a continuum. This treatment may generate some errors in the calculations of mass and energy transfers between the phases [59]. In consideration of this issue and regardless of the limitation of computational resources, the Eulerian-Lagrangian Approach in which each particle is tracked might present more accurate predictions than the Eulerian-Eulerian Approach [91].

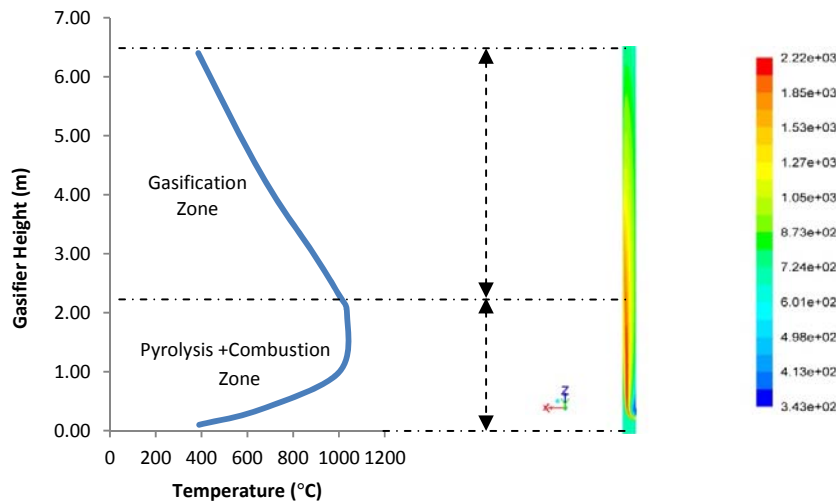


Figure 26: Gasifier Temperature Distribution

3.4.2 Effect of Grid Resolution

In this section, a grids study is implemented to examine the effect of grid resolution on the simulation results. The model initially was built on a grid with 129,621 cells, but the scaled residuals of the solution are higher than the convergence criterion, 2.0×10^{-5} , and the mass imbalance between the inlet and outlet is significant. In order to improve the accuracy of the model, the grid is further refined in the axial direction to generate a grid with 366,249 cells, and all of the residuals for the variables are less than the setting value. Another grid with a higher resolution of 484,833 cells is also produced. The simulation results from these two grids are then compared with each other to check the grid independence for the final solution.

Figure 27 displays the outlet compositions of CO, H₂, CH₄, C₂H₄, and N₂ from the two grids are compared with each other. It can be seen that there is no significant difference between them. The temperature profiles from the two models are also examined. As displayed in Figure 28, the difference between the predicted profiles is insignificant at the heights of 0-4.0 meters where both profiles overlap each other, but at the heights of 4.0-6.5 meters, the temperatures predicted from the grid of 484k-cell are less than those from the grid of 366k-cell. On the other hand, the “wall clock time” for the computation of the 484k-cell grid, 220 hours, is much longer than the time for the 366k-cell grid, 173 hours. Considering the small differences of gas composition and temperature between the two models and shorter computation time for the grid of 366k-cell, the model built on the 366k-cell grid (base case) is then selected for the rest of the analysis.

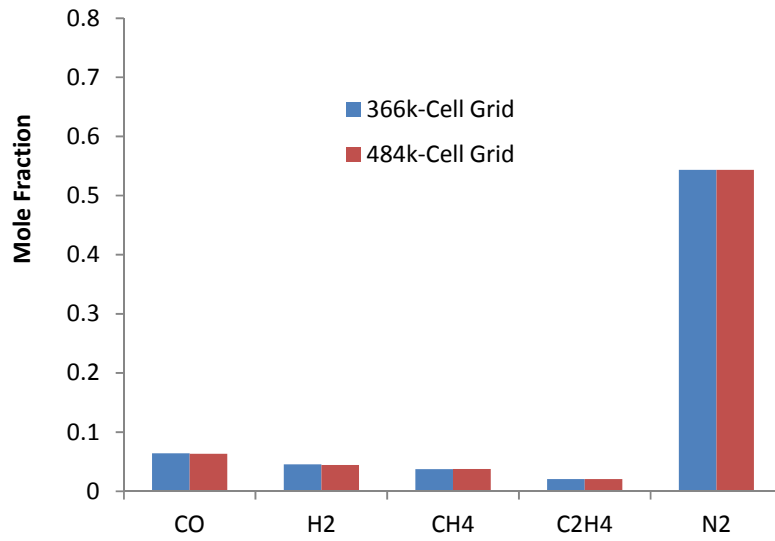


Figure 27: Comparisons of Outlet Gas Compositions from 366k-Cell and 484k-Cell Grids

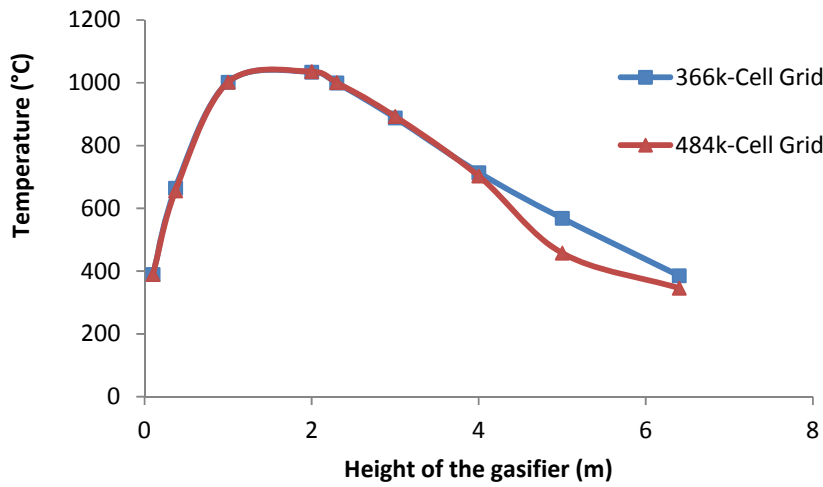


Figure 28: Temperature Comparison of 366k-Cell and 484k-Cell Grids

3.4.3 Comparisons of Turbulence Models

In this section, the gasification models using different turbulence equations including the standard, RNG, and realisable k-epsilon equations are compared with each other to investigate the impact of turbulence models.

The RNG k-epsilon turbulence model is similar to the standard k-epsilon model. However, derived from a robust statistical approach, renormalization group theory, the values of model constants are different from those of the standard k-epsilon model, and an additional term, R_ϵ , is added to the equation of ϵ (turbulent energy dissipation rate). The new features are applied to improve the accuracy and extend the applications of the turbulence model [27, 92]. The detailed explanations of RNG theory and the applications of this model can be found in the work by Orszag et al.[92].

The standard k-epsilon and the RNG k-epsilon models are regarded as semi-empirical models as the equations of dissipation rate, ϵ , are mainly based on some reasonable assumptions, not derived from an exact solution [27]. To tackle this issue and improve the accuracy of turbulence modeling, the realizable k-epsilon model was developed by Shih, et al. [93].

A new model of ϵ was derived from the dynamic equation of the mean-square vorticity fluctuation, and C_μ , a constant for the previous turbulence models, was applied as a variable to build a new formula of eddy viscosity. The realizable k-epsilon model has been proven to be more accurate for simulating the flows with strong streamline curvature and rotations [27]. The detailed descriptions of the equations and theory can be found in the reports by Shih et al.[93] and in Fluent [27].

Figures 29 (a-c) demonstrate the velocity distributions of the gas and solid phases from three turbulence models. As seen in the figures, the air velocity starts to increase in the bottom region, then increases sharply in the lower middle-region, and finally decreases slowly in the upper region near the exit. The respective increase and decrease in the lower middle and upper regions are caused by the temperature changes in these regions of the gasifier. When the temperature rises, the gas velocity increases according to the ideal gas law. Similarly, the gas velocity decreases as the temperature drops. Since the solid phase is dragged by the gas phase, the solid velocity also follows a similar trend.

The differences of velocity distributions between three turbulence models are slight. Based on the similar distributions of gas and solid velocities, the mole fractions of gas

species at the outlet and the axial temperature profile from the different turbulent models are also analogous, as shown in Figures 30 and 31.

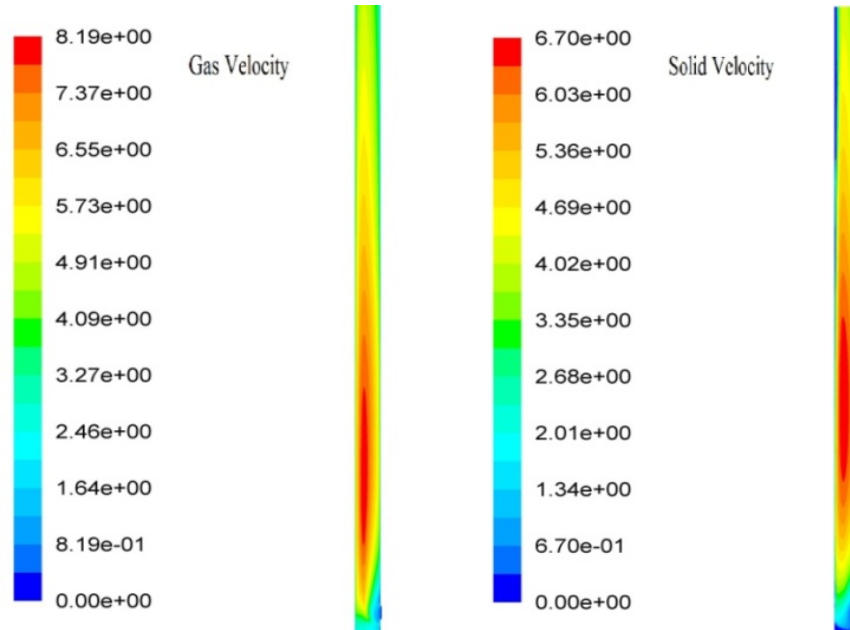


Figure 29 (a): Velocity Distribution of Standard k-epsilon Model

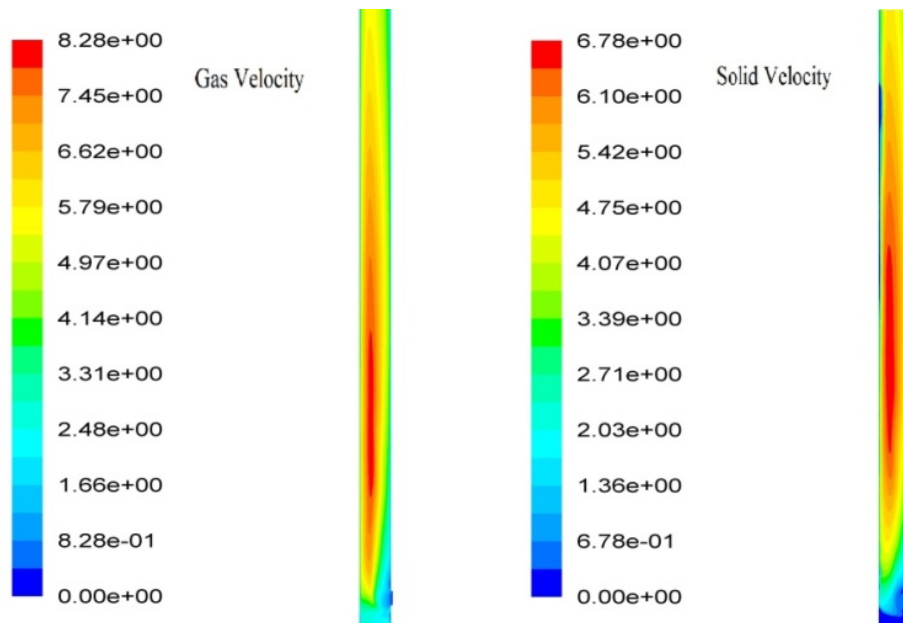


Figure 29 (b): Velocity Distribution of RNG k-epsilon Model

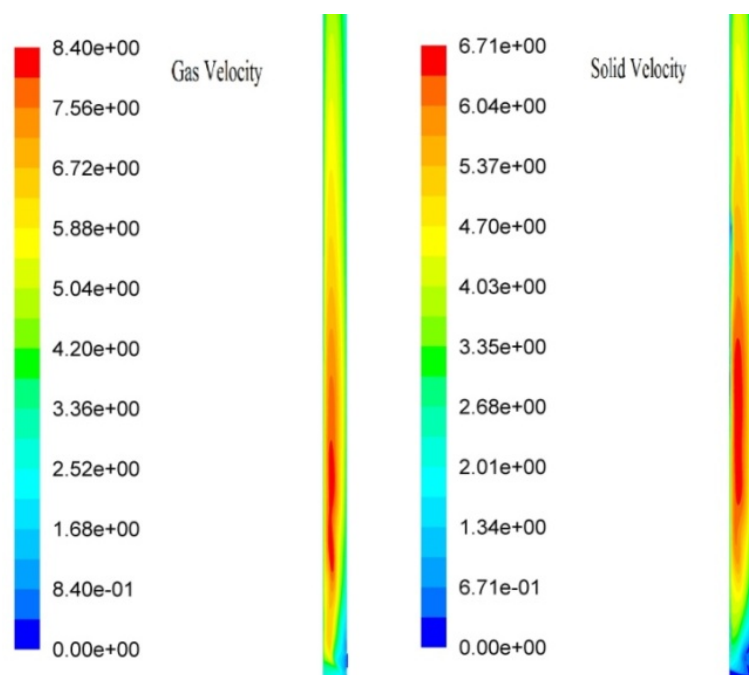


Figure 29 (c): Velocity Distribution of Realizable k-epsilon Model

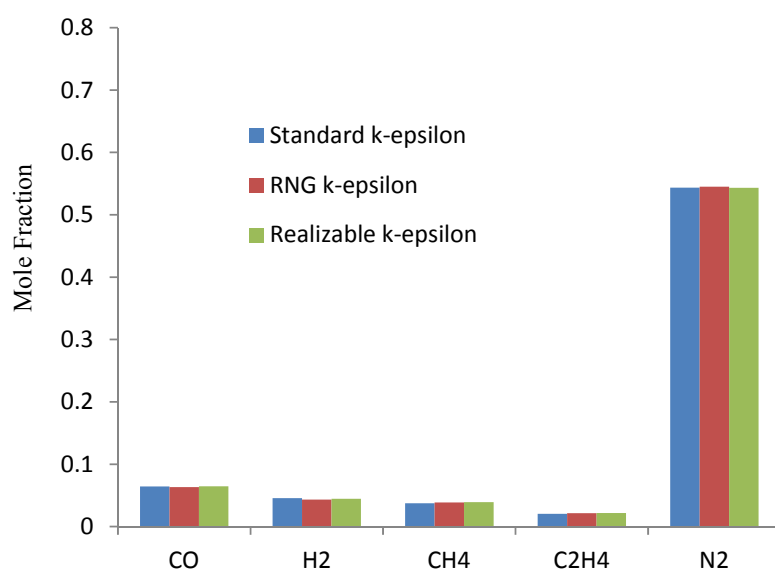


Figure 30: Comparisons of Outlet Gas Compositions from Different Turbulence Models

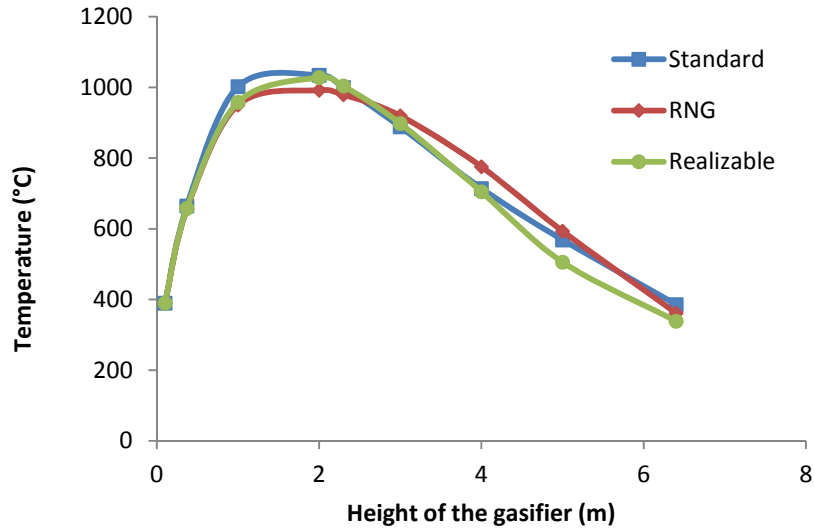


Figure 31: Temperature Comparisons of Turbulence Models

3.4.4 Impact of P-1 Radiation Model

As a major method of heat transfer, thermal radiation plays an important role in the process of gasification. However, under some specific considerations, thermal radiation was not considered in the previous works [60, 62, 66]. As discussed earlier, thermal radiation modeled by the P-1 model is included in our work.

The absorption coefficient, a , is an important factor for the P-1 radiation model. However, there is very limited information about the value of this coefficient, and the value may vary significantly from case to case. As indicated by Hungershoefer, et al. [94], the absorption coefficient of biomass burning aerosol was between $0.12\text{--}0.14\text{ m}^{-1}$, while as reported by Weingartner, et al. [95], the values of this coefficient for soot particles were in the magnitude of $10^{-3}\text{--}10^{-4}\text{ m}^{-1}$. However, considering the fact that the particle diameter in the gasifier is larger than burning aerosol and soot particles, the value of a in the gasifier may then be larger than those of aerosol and soot particles.

In this section, a few of values, 0.5, 1.0, and 5.0 are assigned to the P-1 radiation mode respectively to check the impact of the value of a on the temperature prediction. Meanwhile, the temperature profile predicted from the models using the P-1 modes will

also be compared with the temperature profile from the model without considering thermal radiation to investigate the effect of thermal radiation.

As shown in Figure 32, both profiles follow a similar trend that the temperature increases at the beginning and then decreases after the peak point. However, it is clearly seen that the predicted temperatures from the model without considering thermal radiation are higher than those from the model using the P-1 radiation mode. The peak temperature from the model excluding thermal radiation is, around 1300-1400 °C, much higher than the experimental data [76] and the predicted peak temperature from the model using the radiation mode. The large temperature gap may be caused by neglecting some effect of thermal radiation in the gasifier including the heat radiation within the fluids and the heat loss radiated to the wall. The comparison indicates that the impact of thermal radiation is significant and thermal radiation needs to be included in the gasification model.

On the other hand, as shown in Figure 32, the temperature profiles predicted from the models using different values of a are almost identical and overlay each other. It is shown that the absorption coefficient of solid phase plays a minor role in predicting the gasifier temperature profile. This may be due to the very dilute concentration of solid phase in the gasifier as shown in Figure 22. Additionally, according to our model, the average volume fraction of solid phase in the gasifier is about 0.00038. Therefore, when the light travels through the gasifier that is mostly filled with the gases, over 99%, the radiant energy may be mainly absorbed by the gas phase instead of the solid phase, and then a change of absorption coefficient for the solid phase may be unable to affect the gasifier temperature prediction significantly. For the rest of our study, a value of 1.0 is assigned to the absorption coefficient.

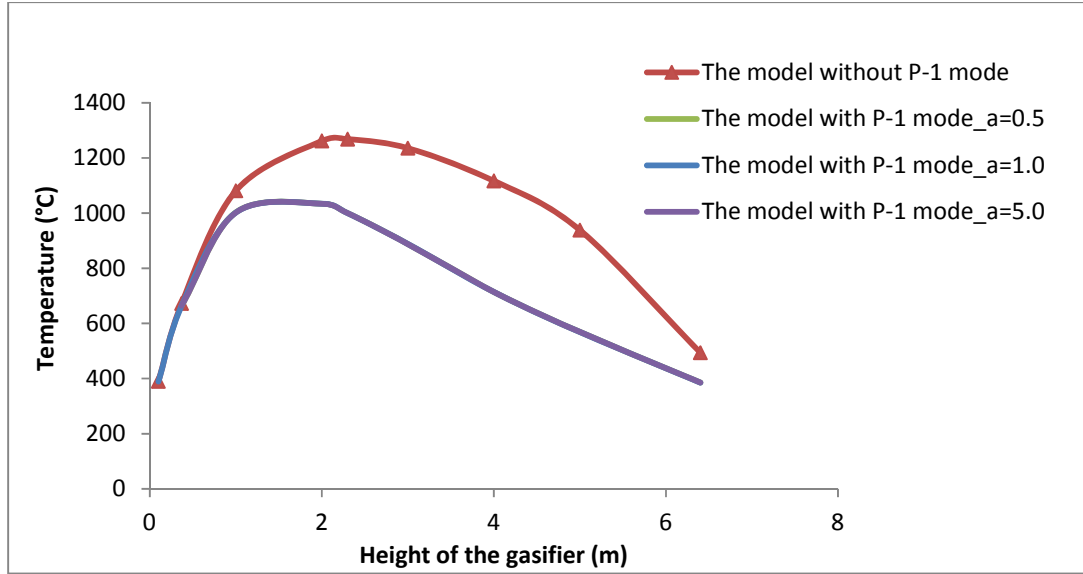


Figure 32: Temperature Comparison of Models with and without P-1 Mode

3.4.5 Effect of Water-Gas Shift (WGS) Reaction

As mentioned earlier, the water-gas shift (WGS) reaction was used in many gasification models. However, since the kinetics of WGS reaction was generally obtained from experiments with catalysts [70, 74, 96], considering the non-catalytic conditions and short reactor residence time in the gasifiers using circulating fluidized bed, the role of this reaction in the process of CFB gasification is still unclear [72].

In this section, a model integrated with the WGS reaction is built to examine the impact of this reaction on the gasification process. As shown in Figure 33, the differences of CO and H₂ compositions between two cases are distinct. The outlet compositions of CH₄ and C₂H₄ from two cases are similar. It is because these two species are mainly generated from the pyrolysis, and the impact of WGS reaction on the two species is slight.

Figures 34 (a-c) demonstrate the mole fraction distributions of H₂, CO, and CO₂ between two cases. Note that for the convenience of comparison the legends in the figures have been adjusted and set in the same range for each species, respectively. As seen in the figures, the mole fractions of H₂ and CO₂ in the case with WGS are higher than the base case whilst the mole fraction of CO is less than the base case as a result of the WGS

reaction. Based on the comparisons, one can see that the impact of WGS reaction is noticeable on the predictions of mole fractions of H_2 and CO.

As Lu and Wang [72], [73], Luan et al.[74], and Gómez-Barea, et al. [75] pointed out, in a real operation of gasifier, the WGS reaction was very far from the equilibrium, and without considering the catalytic characteristics of WGS reaction, applying the WGS reaction kinetics directly in the simulation of gasification might affect the model accuracy. For this work, since no catalyst exists in the gasifier and the reactor residence time is short, the WGS reaction is not included. However, in case the “clean” or non-catalytic kinetic data of WGS reaction is available under the normal operating conditions (not supercritical-water) in the future, we will implement it in our model to gain a better understanding of the role of WGS reaction in gasification.

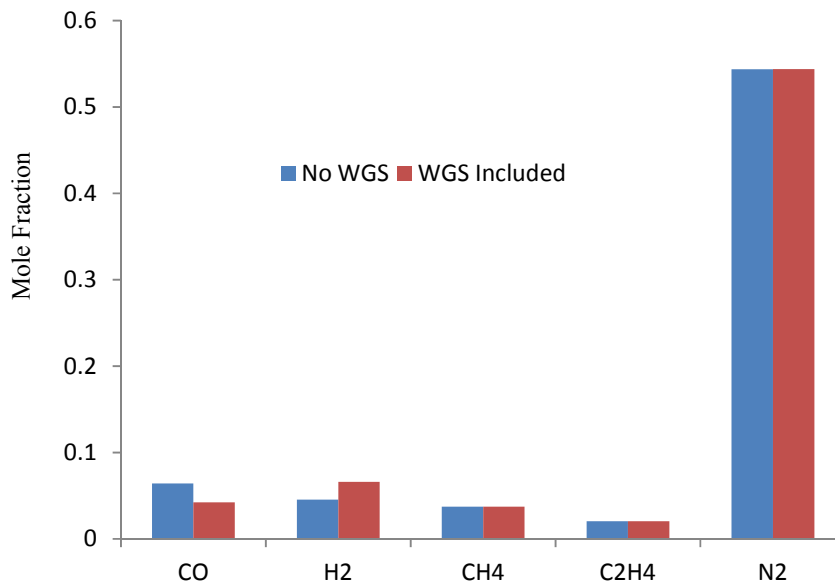


Figure 33: Comparisons of Outlet Gas Compositions from Models using WGS and without WGS

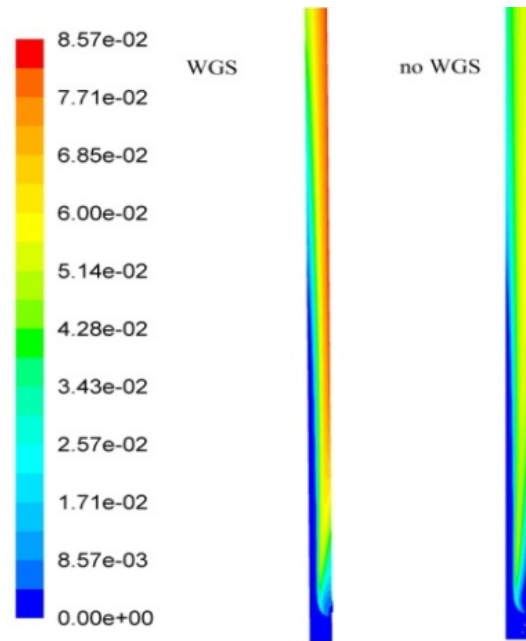


Figure 34 (a): Mole fraction Comparison of H_2

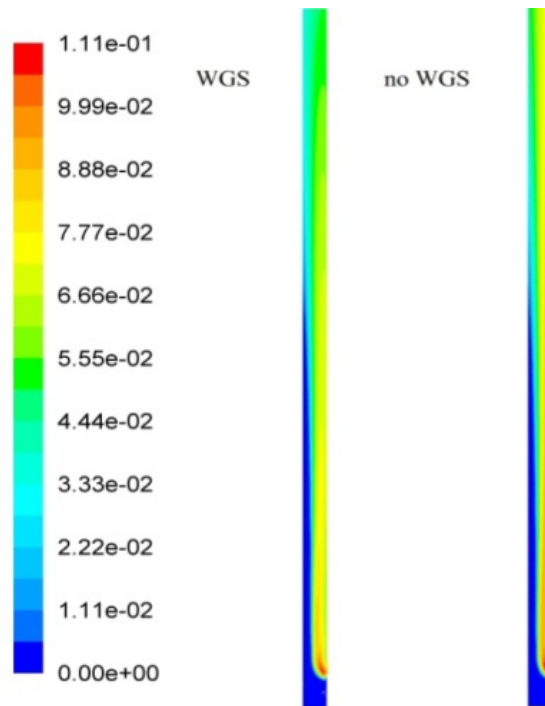


Figure 34 (b): Mole fraction Comparison of CO

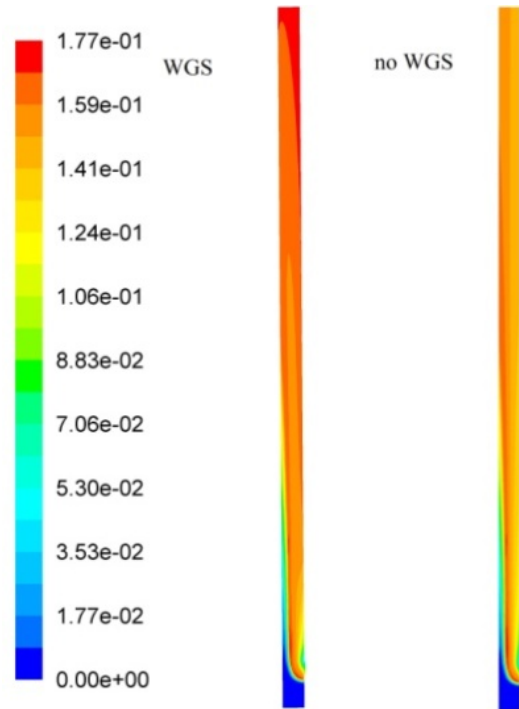


Figure 34 (c): Mole fraction Comparison of CO₂

3.4.6 Studies of Equivalence Ratio (ER)

The equivalence ratio (ER) is defined as the ratio of the amount of air supply for gasification to the stoichiometric amount of air required by combustion. Theoretically, $ER < 1.0$ stands for the conditions of incomplete combustion or gasification (lean air/oxygen), while $ER = 1.0$ means a complete combustion in which the combustible gases such as CO, H₂, CH₄, and C₂H₄ are fully consumed.

As indicated by Gunaratne [97], the contents of combustible gases initially increase with the ER until the ER reaches the optimum value, and after this optimal point, the combustible gas contents decrease as the ER increases. Since the heat of gas combustion is the main energy source for the whole process, the optimum ER is actually the critical point where the heat released from gas combustion matches the maximum energy demand from the rest of the processes (Reactions R1, R3 and R4) and the maximum amount of combustible gases can be generated. After the optimal ER, increasing air or oxygen supply can only burn more combustible gases.

The optimum ER for downdraft gasifiers is reportedly in the range of 0.19-0.43 [97, 98], while for updraft gasifiers such as fluidized-bed gasifiers, the optimum ER is around 0.25, as suggested by Basu [99], [100].

Figure 35 exhibits the mole fractions of combustible gas species (CO, H₂, CH₄, and C₂H₄) from the models using different values of ER. As shown in the figure, the mole fractions of combustible species decrease with the increase of ER. The main reason is that after the optimum ER the combustible species are continuously burned when the amount of air or oxygen increases. As a result of gas combustion, the temperature inside the gasifier also rises as the ER increases, shown in Figure 36. The relationships between gas composition, temperature, and ER discussed above were also found in the report by Zainal et al.[98].

Since the values of ER selected for this analysis, in the range of 0.41-0.60, are larger than the recommended optimum ER, 0.25 [99, 100], the pattern of combustible gas content shown in Figure 35 is actually the part of the trend after the optimum ER. Therefore, the optimum ER and the trend before this point are unseen in this work. The reason small value of ER such as 0.25 is not chosen for this study is that the hydrodynamic regime in the gasifier might change from circulating fluidized bed (CFB) to bubbling fluidized bed (BFB) when small ER as low as 0.25 is applied [75], and the discussion about bubbling fluidized bed is beyond the scope of this work.

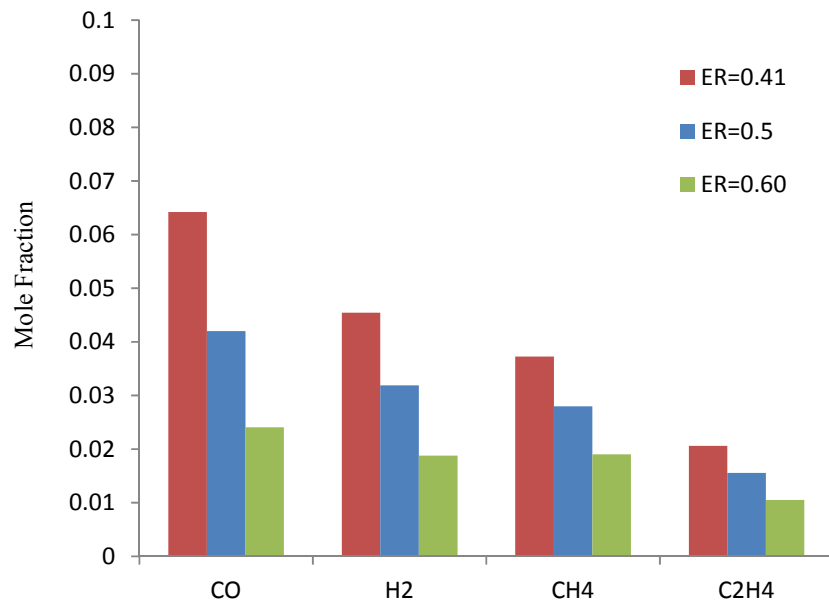


Figure 35: Comparisons of Outlet Gas Compositions from Case Studies using Different ER

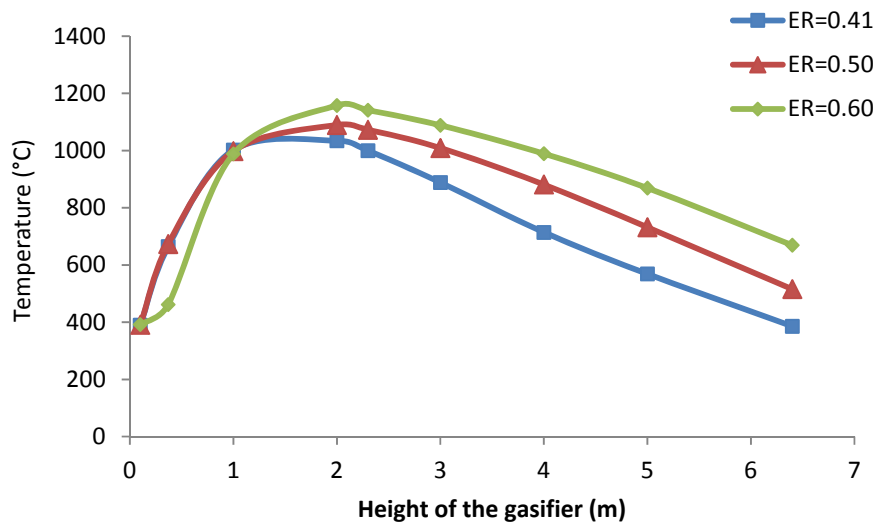


Figure 36: Temperature Profiles of Case Studies Using Different ER

3.5 Conclusions

In this chapter, a 3-D steady-state model was developed to simulate biomass gasification in a CFB reactor. The standard k-epsilon turbulence model was coupled with the kinetic theory of granular flow to describe the hydrodynamics of gas-particle system in the gasifier. The equations of continuity, motion, and energy were integrated with the kinetics of homogeneous and heterogeneous reactions to calculate mass and energy transfer in the gasifier. The simulation results were compared with the experimental data, and a good agreement was observed.

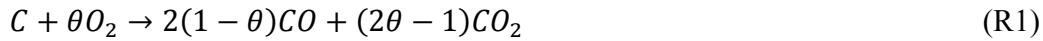
Additionally, a grid study was conducted to examine the grid independence of the solution, and the model built on the 366,249-cell grid was chosen for the rest of the analysis. The impact of turbulence models was also discussed, and it was observed that the difference between the standard k-epsilon, RNG, and the realizable k-epsilon turbulence models was insignificant. The P-1 radiation model was applied to simulate thermal radiation in the gasifier, and the importance of thermal radiation was verified by the comparison of the models with and without the radiation mode. The role of WGS reaction was also investigated, and it was concluded that the reaction of WGS needed to be applied with caution due to the non-catalytic conditions within the gasifier. Finally, various equivalence ratios were applied to test the model, and it was found that the mole fractions of combustible species decreased and the overall temperature in the gasifier increased as the values of ER rose in the selected range.

Chapter 4

Effect of Char Combustion Product Distribution Coefficient on the CFD Simulation of Biomass Gasification in Circulating Fluidized-Bed Reactor

4.1 Introduction

Char combustion is an important reaction in gasification process, and the primary reaction product would be supposedly CO₂. However, a mechanism in which both CO and CO₂ are considered as primary products has been widely accepted [86, 101-106]. A product distribution coefficient of char combustion, θ , is applied to determine the split of reaction products (CO and CO₂) as follows:



If θ is equal to 0.5 or 1.0, the sole gas product is CO or CO₂, respectively. When θ is in the range of 0.5-1.0, both CO and CO₂ are the primary reaction products. The value of θ is determined by many factors such as particle diameter, temperature, carbonaceous material and ash contents, and oxygen partial pressure [107, 108].

Some correlations were developed to determine the ratio of the products. As indicated by Arthu [101], the value of CO/CO₂ was independent of burning time, and air velocity did not affect the ratio until reaction temperature reached 900 °C. Meanwhile, the ratio was found to be exclusively related to reaction temperature, and increased exponentially with temperature. Rajan and Wen [109] proposed that the ratio was determined by both temperature and particle diameter. Du, et al. [110] reported that in addition to reaction temperature, the value of CO/CO₂ was also affected by partial pressure of O₂, and it decreased as oxygen partial pressure increased. Ashman and Mullinger [107] pointed out that CO/CO₂ might vary significantly for different chars or carbons, and the recommended ratio values from the literatures might be specific for the chars tested in the literatures.

For the sake of simplicity, θ is generally treated as a constant rather than a variable for the modeling of biomass or coal gasification. Yan, et al. [111] built a 1D (one-dimensional) steady-state model of coal gasification in a bubbling fluidised bed (BFB), using a prescribed value of 0.8 for θ . In a 2D (two-dimensional) CFD model of coal gasification by Yu, et al. [62], the value of θ was set as 2/3. A constant value of 0.5 was used by Murgia, et al. [66] for char combustion in a CFD model of an air-blown updraft coal gasifier. The same value of θ was also applied in a 3D (three-dimensional) CFD model of gasification in a cross-type two-stage reactor [74]. Despite different values of θ being used, all of the results from the above models were reportedly in good agreement with their experimental data, but it was unclear how the value of θ influences the predictions of gasification model.

Yan, et al. [112] developed a 1D isothermal model of BFB coal gasification. Based on this isothermal model, Yan and Zhang [108] conducted an investigation and concluded that θ with a value between 0.75-0.85 had negligible impact on the predictions of reactor temperature, gas production rate, and gas product composition. However, due to the complex flow pattern in the gasifier, the isothermal hypothesis may not be realistic for a fluidized-bed gasifier. Additionally, the model was built for a bubbling fluidized-bed gasifier, and the conclusion might not be suitable for another type of fluidized-bed gasifier such as circulating fluidized-bed (CFB) gasifier which has a different flow pattern and can present more efficient mass and energy transfer for gasification [56].

In this paper, a 3D unsteady-state model is built for the simulation of biomass gasification in a CFB reactor. The RNG (Re-Normalisation Group) k-epsilon turbulence model is integrated with the continuity, momentum, and energy equations to simulate biomass gasification. The predicted distributions of gas composition is validated by experimental data [76], and various values of θ will be applied to investigate the impact of θ on the predictions of gas composition, temperature, and reaction rates in the gasifier. The effect of θ will be further examined by increasing air supply to the gasifier.

4.2 Governing Equations

The governing equations for the 3D unsteady-state model are described as follows:

4.2.1 Conservation of Mass and Momentum

The mass and momentum conservation equations are described by Equations 47-50. The kinetic theory of granular flow is again applied to model the hydrodynamics of the gasifier, and for further details, please refer to Chapter 2.

4.2.2 RNG (Re-Normalisation Group) k-epsilon turbulence model

The RNG k-epsilon turbulence model for the gas phase is shown as follows [27, 92, 113]:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g k_g) + \nabla \cdot (\alpha_g \rho_g v_g k_g) = \nabla \cdot (\alpha_g \alpha_k \mu_{eff,g} \nabla k_g) + \alpha_g G_{k,g} + G_{b,g} - \alpha_g \rho_g \varepsilon_g \quad (69)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_g \rho_g \varepsilon_g) + \nabla \cdot (\alpha_g \rho_g v_g \varepsilon_g) = & \nabla \cdot (\alpha_g \alpha_\varepsilon \mu_{eff,g} \nabla \varepsilon_g) + \frac{\varepsilon_g}{k_g} [C_{1\varepsilon} \alpha_g G_{k,g} - C_{2\varepsilon} \alpha_g \rho_g \varepsilon_g + \\ & C_{3\varepsilon} G_{b,g}] - \alpha_g R_\varepsilon \end{aligned} \quad (70)$$

where μ_{eff} is the effective viscosity, G_k is the generation of turbulence kinetic energy due to the mean velocity gradients, G_b stands for the generation of turbulence kinetic energy due to buoyancy, and R_ε is a new term, derived from the RNG theory. C_μ , $C_{1\varepsilon}$ and $C_{2\varepsilon}$ are 0.0845, 1.42 and 1.68, respectively, based on the analytical solution of RNG theory. The same turbulence model is also applied to the solid phase.

α_k and α_ε are calculated by the following equation:

$$\left| \frac{\alpha - 1.3929}{\alpha_0 - 1.3929} \right|^{0.6321} \left| \frac{\alpha + 2.3929}{\alpha_0 + 2.3929} \right|^{0.3679} = \frac{\mu}{\mu_{eff}} \quad (71)$$

where $\alpha_0 = 1.0$.

4.2.3 Conservation of Energy

The conservation of energy equations for the gas and solid phases are [26, 27]:

$$\frac{\partial \alpha_g \rho_g H_g}{\partial t} + \nabla \cdot (\alpha_g \rho_g v_g H_g) = -\alpha_g \frac{\partial p_g}{\partial t} + \tau_g : \nabla v_g + \nabla \cdot (\alpha_g k_{eff,g} \nabla T_g) + S_g + Q_{gs} \quad (72)$$

$$\frac{\partial \alpha_s \rho_s H_s}{\partial t} + \nabla \cdot (\alpha_s \rho_s v_s H_s) = -\alpha_s \frac{\partial p_s}{\partial t} + \tau_s : \nabla v_s + \nabla \cdot (\alpha_s k_{eff,s} \nabla T_s) + S_s + Q_{sg} \quad (73)$$

where H is the specific enthalpy of the phase, k_{eff} is the effective thermal conductivity, S is the source enthalpy owing to chemical reactions and thermal radiation, and Q is the intensity of heat transfer between the gas and solid phases.

k_{eff} , the effective thermal conductivity, is defined as follows:

$$k_{eff} = \alpha_{eff,t} C_p \mu_{eff} \quad (74)$$

$\alpha_{eff,t}$ is calculated by Equation-9 with $\alpha_0 = \frac{k}{\mu C_p}$, where k is the thermal conductivity, and C_p is the heat capacity.

The enthalpy source from thermal radiation is computed by the P-1 model [27, 79], as defined by Equation 57-59 in Chapter 3.

The intensity of heat exchange between the phases is calculated by the model of Gunn [78], as defined by Equations 54-56 in Chapter 3.

4.2.4 Conservation of Mass Species

The conservation of mass species equation for the gas phase is [26, 27]:

$$\frac{\partial (\rho_g \alpha_g Y_{i,g})}{\partial t} + \nabla \cdot (\rho_g \alpha_g v_g Y_{i,g}) = -\nabla \cdot (\alpha_g J_{i,g}) + \alpha_g R_{i,g} + R \quad (75)$$

$$J_{i,g} = -(\alpha_{eff,m} \mu^t) \nabla Y_{i,g} - D_{T,i} \frac{\nabla T}{T} \quad (76)$$

where $\alpha_{eff,m}$ is calculated by Equation-9 with $\alpha_0 = \frac{1}{Sc}$, where Sc is the molecular Schmidt number.

4.2.5 Heterogeneous and Homogeneous Reactions

As biomass particles are fed into the gasifier, volatiles and char are first generated from biomass pyrolysis. The volatiles are partially burned in the limited amount of O_2 , and the heat of combustion is provided to other chemical reactions. Char also reacts with O_2 , and when O_2 is depleted, the residual char reacts with CO_2 , H_2O (water vapor), and H_2

respectively to generate CO, H₂, and CH₄. The gases in the gasifier can also react with each other to generate other gases.

For the current study, the following chemical processes are included in the model: biomass pyrolysis, heterogeneous reactions of char, and homogeneous gas-phase reactions. The kinetic data of biomass pyrolysis, char reactions, and gas-phase reactions are listed in Table 6.

Table 6: Kinetic Data of Chemical Reactions

Pyrolysis of Biomass [82]		
Biomass → Char + Ash + Moisture + Volatile (CO, CO ₂ , CH ₄ , C ₂ H ₄ , H ₂ O)		$r_p = k_p C_{char}$, $k_p = f A T^n \exp\left(-\frac{E_a}{RT}\right)$ $f = 1.51 \times 10^3$, $n = -1.2$, $A = 99.0 \text{ s}^{-1}$, $E_a = 11.14 \text{ kJ/mol}$
Heterogeneous Char Reactions [84, 85]		
Diffusion and Kinetic controlled model		
$r_{heter,i} = \frac{6V\alpha_s}{d_p} \cdot \frac{P_i}{\left(\frac{1}{k_{diff,i}} + \frac{MW_C}{k_{kinet,i}}\right)}$, $k_{diff,i} = \frac{D_i Sh}{RT d_p}$, $Sh = 2 + 0.6 Re^{\frac{1}{2}} Sc^{\frac{1}{3}}$, $k_{kinet,i} = A_i \exp\left(-\frac{E_i}{RT}\right)$ where V is the volume of char particles, A is the pre-exponential factor, E is the activation energy, and MW_C is the molecular weight of char.		
$C + \theta O_2 \rightarrow 2(1 - \theta)CO + (2\theta - 1)CO_2$ (R2)		$k_{kinet,C+O_2} = 2.0 \times 10^{-2} \exp\left(-\frac{3000}{T}\right)$
$C + CO_2 \rightarrow 2CO$ (R3)		$k_{kinet,C+CO_2} = 6.35 \times 10^{-3} \exp\left(-\frac{19500}{T}\right)$
$C + H_2O \rightarrow CO + H_2$ (R4)		$k_{kinet,C+H_2O} = 2.0 \times 10^{-2} \exp\left(-\frac{8240}{T}\right)$
$C + 2H_2 \rightarrow CH_4$ (R5)		$k_{kinet,C+H_2O} = 1.18 \times 10^{-5} \exp\left(-\frac{17921}{T}\right)$
Homogeneous Reactions [87, 114-117]		
$CO + 0.5O_2 \rightarrow CO_2$ (R6)		$r_{CO} =$ $1.30 \times$ $10^{11} \exp\left(-\frac{126 \text{ kJ/mol}}{RT}\right) [CO][O_2]^{0.5} [H_2O]^{0.5}$
$H_2 + 0.5O_2 \rightarrow H_2O$ (R7)		$r_{H_2} = 2.20 \times 10^9 \exp\left(-\frac{109 \text{ kJ/mol}}{RT}\right) [H_2][O_2]$
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ (R8)		$r_{CH_4} =$ $5.01 \times 10^{11} \exp\left(-\frac{203 \text{ kJ/mol}}{RT}\right) [CH_4]^{0.7} [O_2]^{0.8}$
$C_2H_4 + O_2 \rightarrow 2CO + 2H_2$ (R9)		$r_{C_2H_4} =$ $1.0 \times 10^{12} \exp\left(-\frac{173 \text{ kJ/mol}}{RT}\right) [C_2H_4][O_2]$

4.2.6 Enhanced Wall Treatment

The standard wall functions were not used in this model, due to the limitations of wall functions as described in our previous study. In this model, a near-wall treatment approach, called “enhanced wall treatment” is applied and coupled with the RNG k-epsilon turbulence model. The enhanced wall treatment can solve the entire viscosity-affected near-wall region, and the validity of near-wall modeling is extended from the log-law region to the viscous sublayer. This near-wall treatment generally consists of the enhanced wall treatment of ε and momentum equations [27].

The enhanced wall treatment of ε equation is applied to both the viscous affected regions and the fully turbulent region. In the viscous affected region ($Re_y < 200$, where $Re_y \equiv \frac{\rho y \sqrt{k}}{\mu}$), the equation of ε is not used, while the equations of momentum and k still remains as is. Meanwhile, in the fully turbulent region ($Re_y > 200$), all of the momentum, k , and ε equations are retained. The turbulent viscosity in the near-wall region, μ_{enh}^t , is defined by a smooth function as follows [27, 118]:

$$\mu_{enh}^t = \lambda_\varepsilon \mu^t + (1 - \lambda_\varepsilon) \mu_{2layer}^t \quad (77)$$

$$\mu_{2layer}^t = \rho C_\mu l_\mu \sqrt{k} \quad (78)$$

$$\lambda_\varepsilon = \frac{1}{2} \left[1 + \tanh \left(\frac{Re_y - 200}{A} \right) \right] \quad (79)$$

$$A = \frac{|\Delta Re_y|}{\text{artanh}(0.98)} \quad (80)$$

where l_μ is the length scale, y is the normal distance between the cell center and the wall, and ΔRe_y is a prescribed value.

The enhanced wall treatment for the momentum equation is as follows [27, 118] :

$$v^+ = e^\Gamma v_{lam}^+ + e^{1/\Gamma} v_{turb}^+ \quad (81)$$

$$\Gamma = -\frac{a(y^+)^4}{1+by^+} \quad (82)$$

$$y^+ \equiv \frac{\rho u_\tau y}{\mu} \quad (83)$$

where $a=0.01$, $b=5$, u_τ is the friction velocity, and v^+ , v^+_{lam} , and v^+_{turb} are the normalized velocities for the near-wall, laminar, and turbulent regions, respectively. For further details, the reader is referred to the report by Kader [118].

4.3 Set-up of Numerical Experiments

A 3D unsteady-state CFD model is built in ANSYS Fluent 14.0, and a schematic diagram of the gasifier is shown in Figure 37, which is similar to the experimental gasifier used by García-Ibañez, et al. [76]. The properties of biomass sample used in the experiment are listed in Table 7. Different values, 0.50, 0.75, and 1.0, are assigned to the product distribution coefficient of char combustion, θ . The simulation results including the profiles of gas composition and gasifier temperature from the models using different air flow rate are compared with each other to investigate the impact of θ on the CFD modeling of biomass gasification in a CFB reactor. As shown in Table 8, nine cases are set up to conduct the investigation.

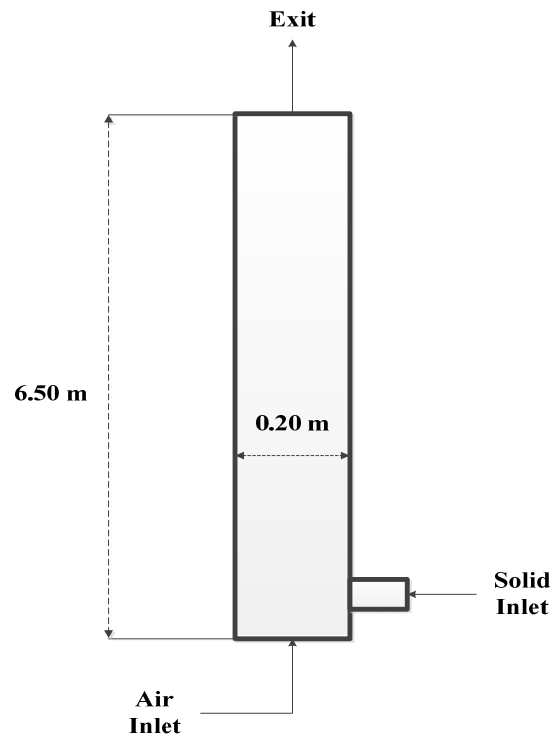


Figure 37: Schematic Diagram of Gasifier

Table 7: Biomass Sample Properties

Moisture (wt%)	Density (kg/m ³)	Proximate Analysis (dry basis)			Ultimate Analysis (d.a.f basis)			
		VM	FC	ASH	C	H	O	others
8.9	659	74.4	17.1	8.5	52.7	7.2	38.1	2.0

VM: Volatile Matter; FC: Fixed Carbon; ASH: ash; d.a.f: dry ash free

Table 8: Set-up of Case Studies for the coefficient, θ

Air Flow Rate (Nm ³ /h)	$\theta = 0.50$	$\theta = 0.75$	$\theta = 1.0$
109	Case 1	Case 2	Case 3
120	Case 4	Case 5	Case 6
147	Case 7	Case 8	Case 9

The mathematical model is solved using the finite control volume method, and the scheme of phase coupled SIMPLE is used for the coupling of pressure and velocity. The convergence criterions, absolute scaled residual, are set as 1.0×10^{-3} for the continuity equation and 1.0×10^{-4} for other equations; however, in the computation, all of the equations reach the converged solutions under 1.0×10^{-4} . In order to reach a converged solution stably and quickly, a steady-state solution is first achieved with the same settings, and the unsteady-state solution is then developed from it in a period of 30-second real time. The time of computation for each test is about 8-9 days on a cluster of 12 CPU nodes at 2.9 GHz.

4.4 Results and Discussion

4.4.1 Impact of θ on Outlet Gas Composition Predictions (Cases 1-3)

In this study, case 3 is set as a base case. As displayed in Figures 38, the predicted outlet gas compositions are in a good agreement with the experimental data [76]. Additionally, Figure 39 (a) shows that the temperature profile from case 3 can accurately predict the reaction zone of pyrolysis and combustion between 0-2.3 meters, and the zone of gasification between 2.3-6.5 meters, which match with the findings by García-Ibañez, et al. [76]. Since the simulation results from case 3 are very similar to those of the model described in Chapter 3, for the simplification of this work, the reader is referred to Chapter 3 to find further details of model validation.

Figure 38 demonstrates the outlet gas compositions predicted from cases 1-3. As seen in this figure, the difference between the predictions of gas compositions from the models using different values of θ is insignificant. Therefore, it might show that the char gasification production coefficient, θ , has minor impact on the predictions of outlet gas composition as proposed by Yan and Zhang [108]. It may be because in the modeling of biomass gasification, the outlet gas compositions are not just determined by char combustion, other reactions such as biomass pyrolysis, gas combustion, and the reaction of char and water vapor may also play important roles in the gas production [108]. Accordingly, a change of θ may not be able to cause significant impact on the predictions of outlet gas compositions.

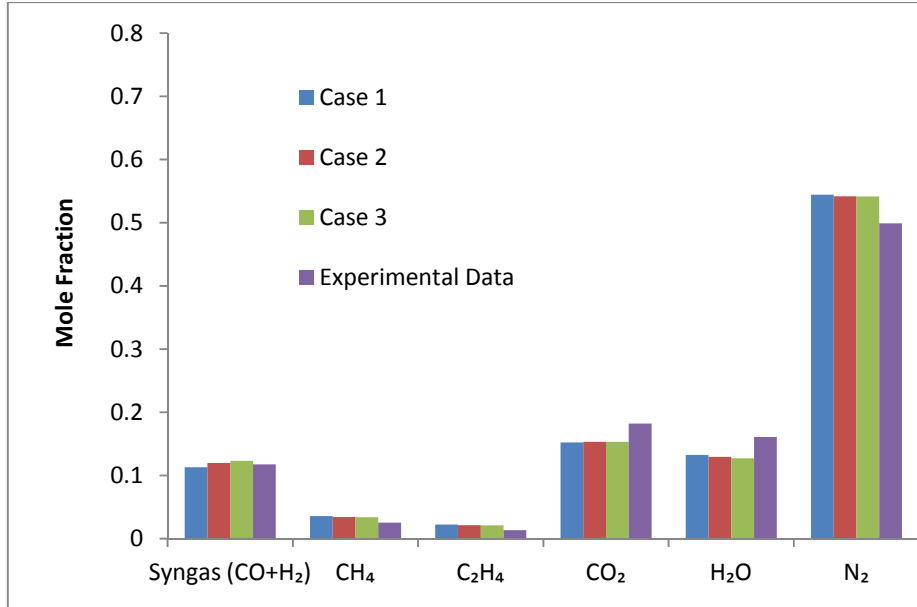


Figure 38: Comparison of Predicted Outlet Gas Composition and Experimental Data

4.4.2 Impact of θ on Gasifier Temperature Distribution (Cases 1-3)

Figures 39 (a) and (b) demonstrates the temperature profiles predicted from cases 1-3. As seen in Figure 39 (a), for case 1, the gasifier temperature increases sharply, up to about 1200 °C, between the heights of 0-1.0 meter, and then decreases along the height of the gasifier. The temperature profiles of cases 2 and 3 overlap each other. The temperatures for the two cases first increase quickly in the bottom region, then reach a plateau, around 1000 °C, between the heights of 1.0-2.3 meters, and finally decrease slowly along the gasifier. As demonstrated in Figure 39 (b), the high temperature area from case 1 is much shorter than those of cases 2 and 3.

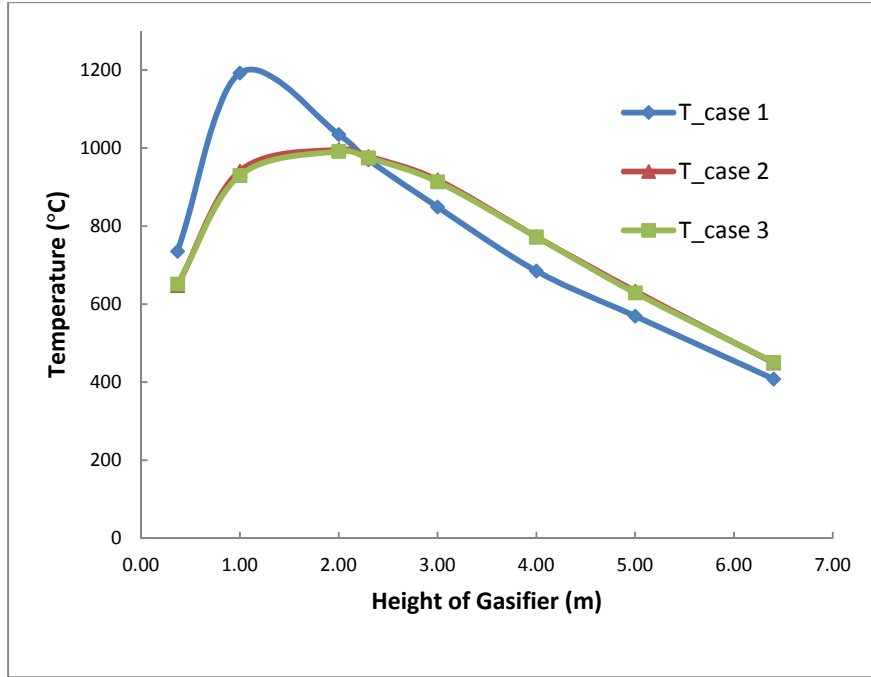


Figure 39 (a): Temperature Profiles from Cases 1-3

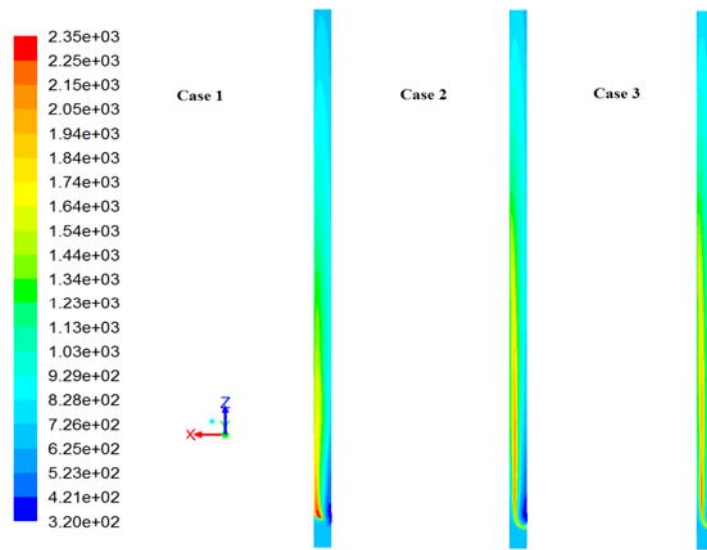


Figure 39 (b): Temperature Contours on XZ Plane (Cases 1-3)

From the comparison above, it is observed that the value of θ can influence the predicted temperature profile. The reactor temperature for the case 1 in which θ is set as 0.5 increases more rapidly in the lower region of the gasifier than those in cases 2 and 3 in

which the values of θ are 0.75 and 1.0, respectively. It may be caused by the different stoichiometric coefficients of char combustion and the consequent changes of reaction rates.

In case 1, due to the setting of θ , only 0.5 mole of O_2 is consumed in char combustion. So, compared with cases 2 and 3, there would be more remaining O_2 for the combustion of some gases such as CH_4 , C_2H_4 , and syngas ($CO+H_2$). Since gas combustion can generally happen more rapidly, the temperature may also increase dramatically in a very short period of time. Accordingly, a high peak temperature may then be predicted from case 1, as shown in Figure 39 (a). However, since only a limited amount of air or O_2 is supplied to the gasifier, and after O_2 is depleted, the reactor temperature then starts to drop.

As shown in Figures 40-42, between the heights of 0-1.0 meter, CO , CH_4 , and C_2H_4 combustion reactions in case 1 are much faster than those of cases 2 and 3. On the other hand, it is also seen that between the heights of 1.0-4.0 meters, the rates of reaction R6, 8, and 9 predicted from case 1 are eventually exceeded by those in cases 2 and 3 due to the depletion of O_2 . Consequently, as shown in Figure 39 (a), the temperature of case 1 then decreases more quickly than the temperatures in cases 2 and 3 in the same region of the gasifier, as shown in Figure 39 (a).

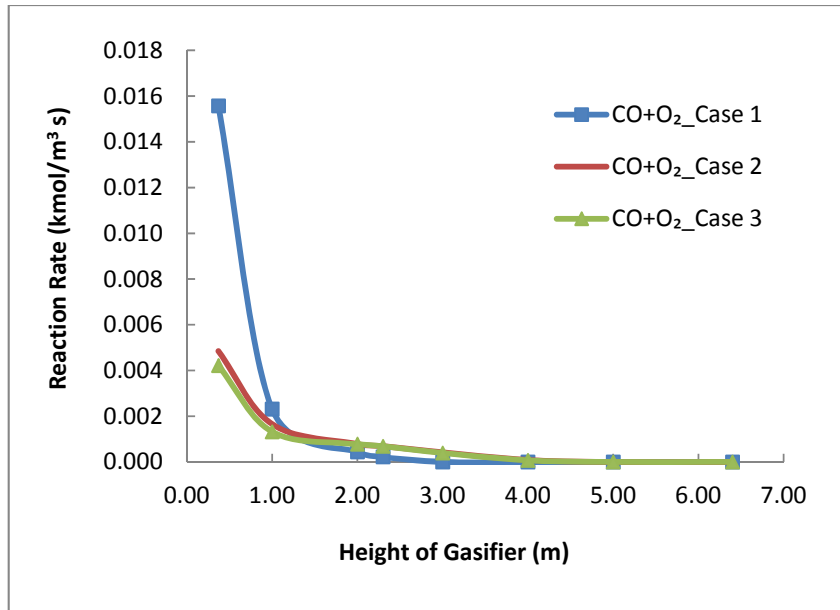


Figure 40: Reaction Rates of CO Combustion in Cases 1-3

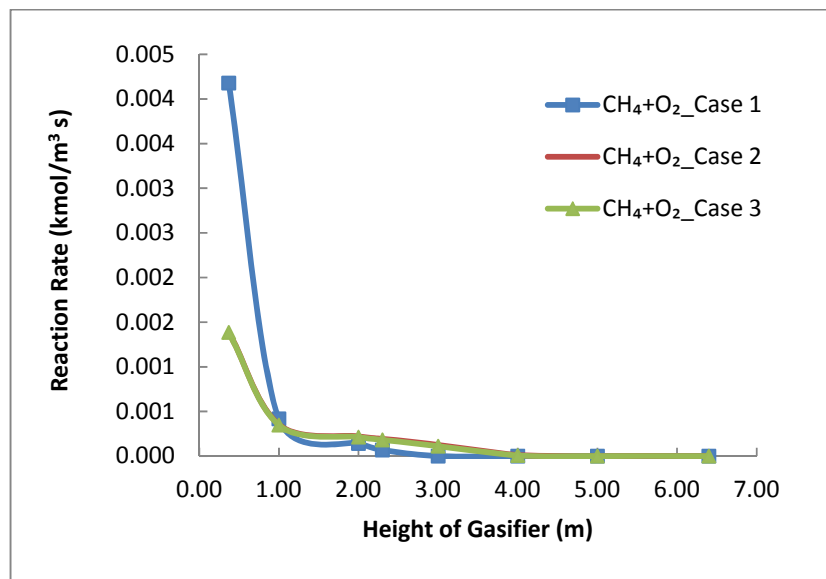


Figure 41: Reaction Rates of CH₄ Combustion in Cases 1-3

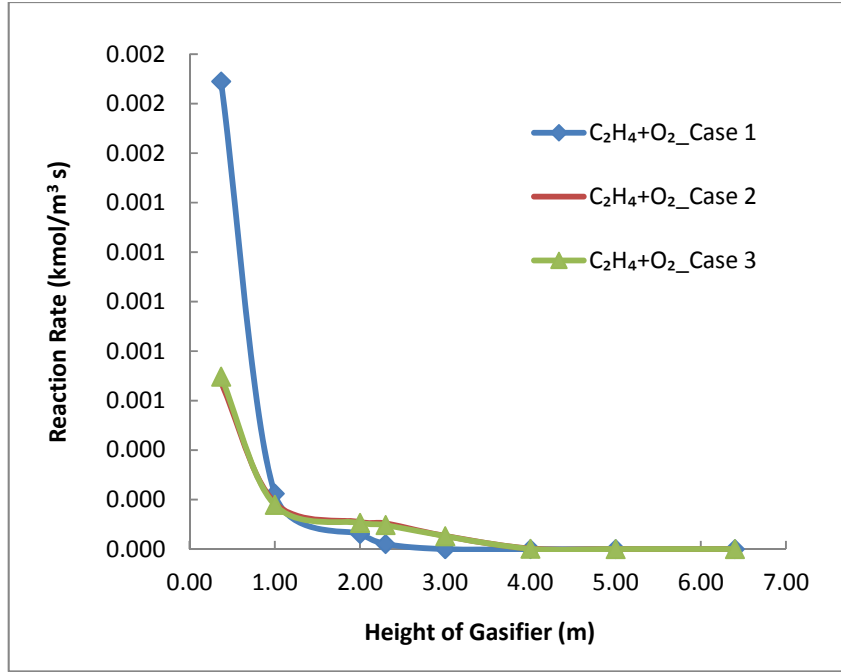


Figure 42: Reaction Rates of C₂H₄ Combustion in Cases 1-3

As displayed in Figure 39 (a), the temperature profiles from cases 2 and 3 with $\theta = 0.75$ and $\theta = 1.0$ respectively, are very similar to each other. In order to further examine the effect of θ on the prediction of gasifier temperature, two additional cases with $\theta = 0.55$ and $\theta = 0.60$, respectively, are added to the current study. Figure 43 clearly presents a transition of gasifier temperature. The high temperature region moves upwards while the value of θ increases from 0.5 to 1.0; meanwhile, the peak temperature decreases, and a plateau of temperature is also formed accordingly.

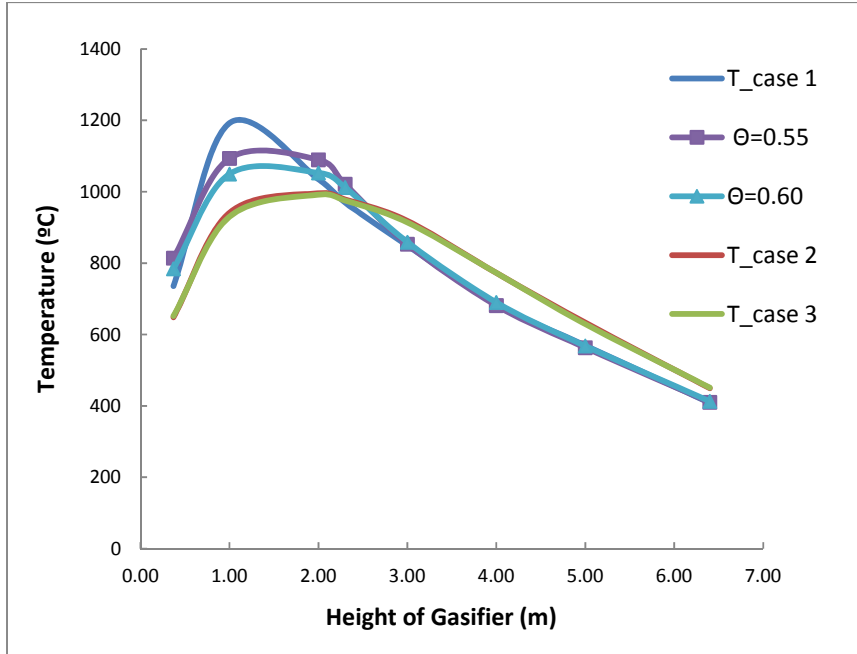


Figure 43: Temperature Profiles from the Cases using Different Values of θ

4.4.3 Impact of θ on Gas Composition Distributions (Cases 1-3)

Since reaction rates vary with temperatures, the cases that predict different temperature profiles may also present different gas composition patterns. Therefore, it is necessary to examine the effect of θ on the gas composition distribution.

In Figure 44, it is observed that O_2 in case 1 is consumed more rapidly in the bottom region of the gasifier than those in cases 2 and 3 due to faster reaction rates. In the meantime, as a main product of gas combustion, CO_2 in case 1 is also generated faster in the same region, as displayed in Figure 45.

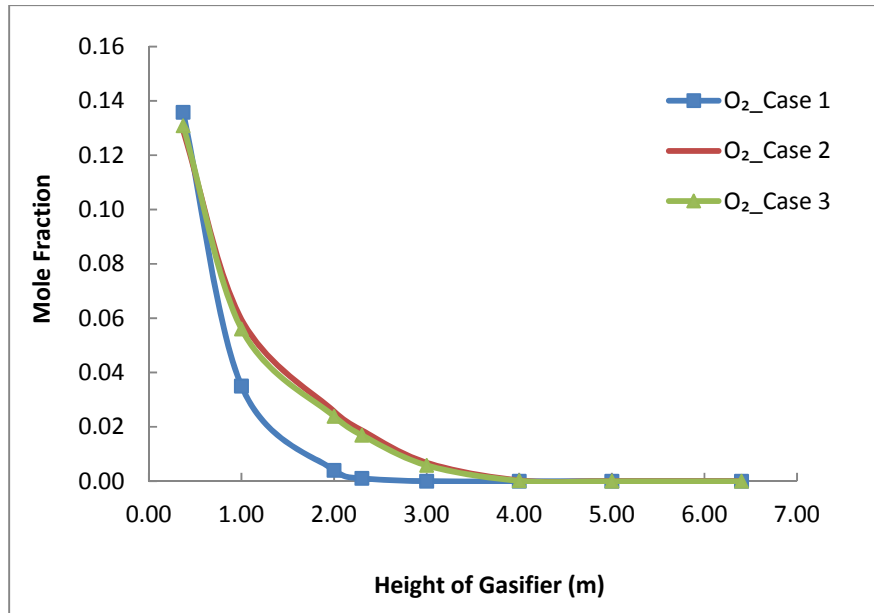


Figure 44: O₂ Distribution inside the Gasifier (Cases 1-3)

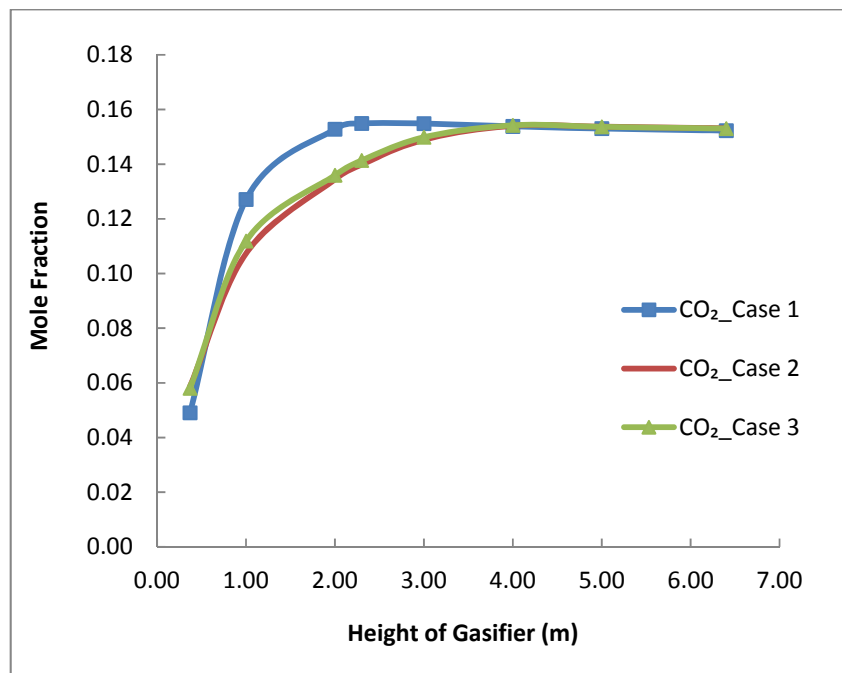


Figure 45: CO₂ Distribution inside the Gasifier (Cases 1-3)

Figures 46 and 47 demonstrate the distributions of CH₄ and C₂H₄ for cases 1-3. As shown in the figures, the gas compositions from cases 1-3 increase in the bottom area due to biomass pyrolysis, then gradually drop due to gas combustion reactions, and finally reach

a constant value when O_2 is depleted in the gasifier. On the other hand, it is also seen that in the bottom region of the gasifier, the compositions of CH_4 and C_2H_4 from case 1 are lower than those of cases 2 and 3 and it may be caused by the faster combustion rates predicted from case 1. However, when O_2 is depleted in the middle region of the gasifier, the gas compositions finally reach constant values and come close to the predictions of cases 2 and 3.

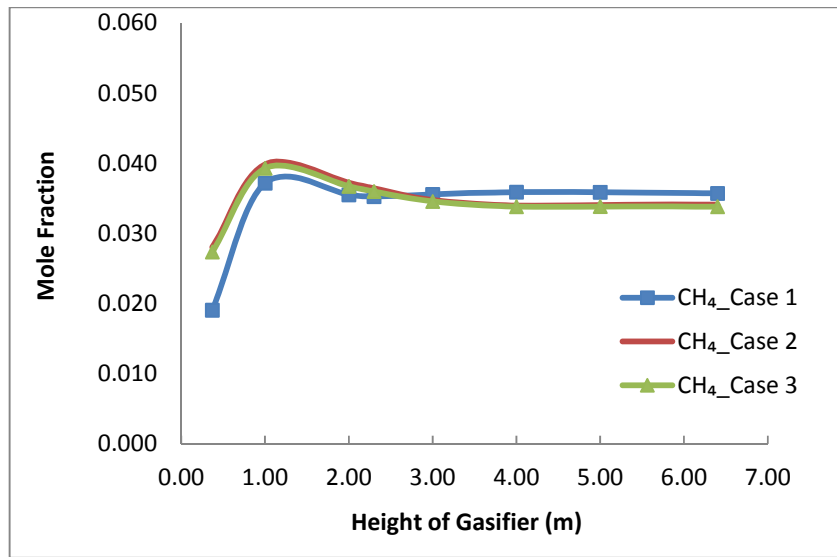


Figure 46: CH_4 Distribution inside the Gasifier (Cases 1-3)

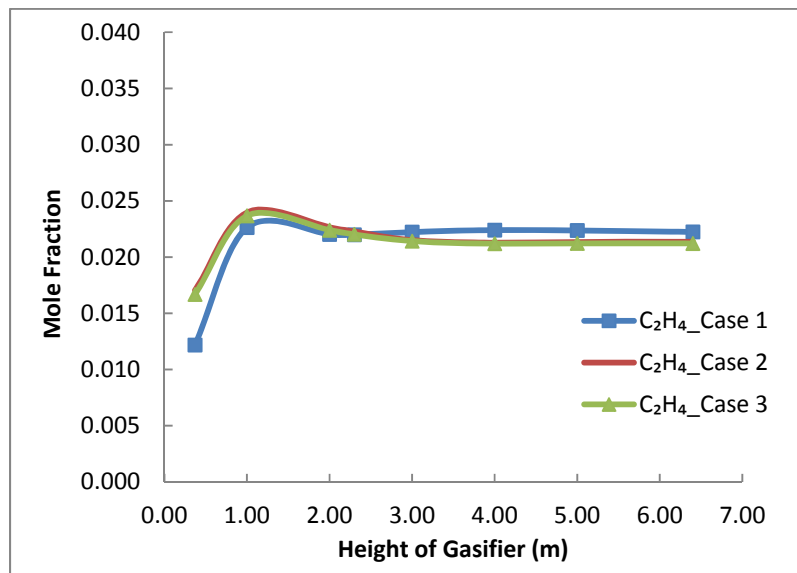


Figure 47: C_2H_4 Distribution inside the Gasifier (Cases 1-3)

Figure 48 demonstrates the distributions of syngas ($\text{CO}+\text{H}_2$) for cases 1-3. As displayed in the figure, the amount of syngas generated from case 1 is less than that of case 1. This may be caused by the different temperature profiles predicted from the cases. In a gasifier, syngas is mainly generated from the reaction of char and water vapor (reaction R4) which generally occurs in the middle and upper regions of the gasifier. As shown in Figure 39 (a), for case 1, the temperatures between the heights of 2.3-6.5 meters are lower than those of cases 2 and 3, and consequently, the rates of reaction R4 may also be lower than the rates of cases 2 and 3. Thus, due to the slower reaction rate of R4 in these regions, lower syngas composition predictions for case 1 may then be observed in Figure 48.

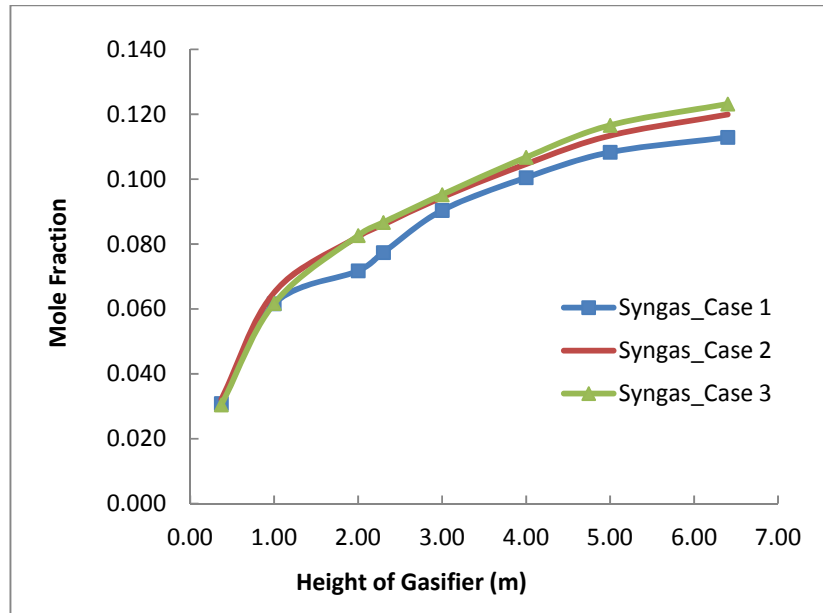


Figure 48: Syngas Distribution inside the Gasifier (Cases 1-3)

It is noted that although the cases using various values of θ present different temperature and gas composition profiles, the difference between the predictions of outlet gas compositions is still small. It is mainly because apart from char combustion, other reactions such as pyrolysis and the reaction of char and water vapor (R4) also play important roles in the gas production. Varying the value of θ for char combustion may affect the distribution of gas composition to some extent, but it might not be able to cause significant impact on the predictions of outlet gas compositions.

4.4.4 Effect of Air Flow Rate (Cases 4-9)

In this section, case studies using different air flow rates (cases 4-6, and 7-9) are implemented to further examine the impact of θ on the predictions of gas composition and reactor temperature.

Figures 49 and 50 demonstrate the predictions of outlet gas compositions for cases 4-6 (air flow rate: 120 Nm³/h), and 7-9 (air flow rate: 147 Nm³/h), respectively. It is observed that the differences between the outlet gas compositions from the cases using different values of θ are insignificant. It therefore confirms the conclusion of Section 4.4.1 that the coefficient of θ has a minor influence on the predictions of outlet gas compositions.

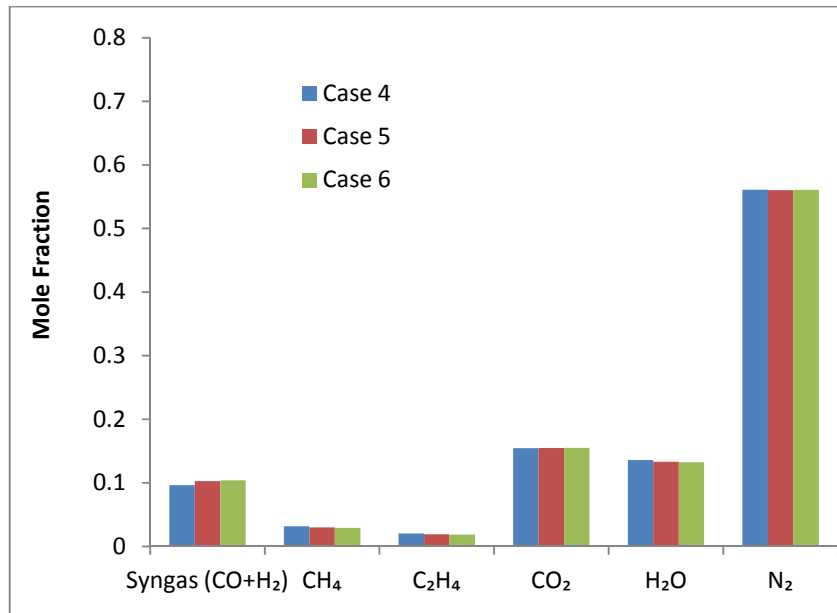


Figure 49: Outlet Gas Compositions from Cases 4-6

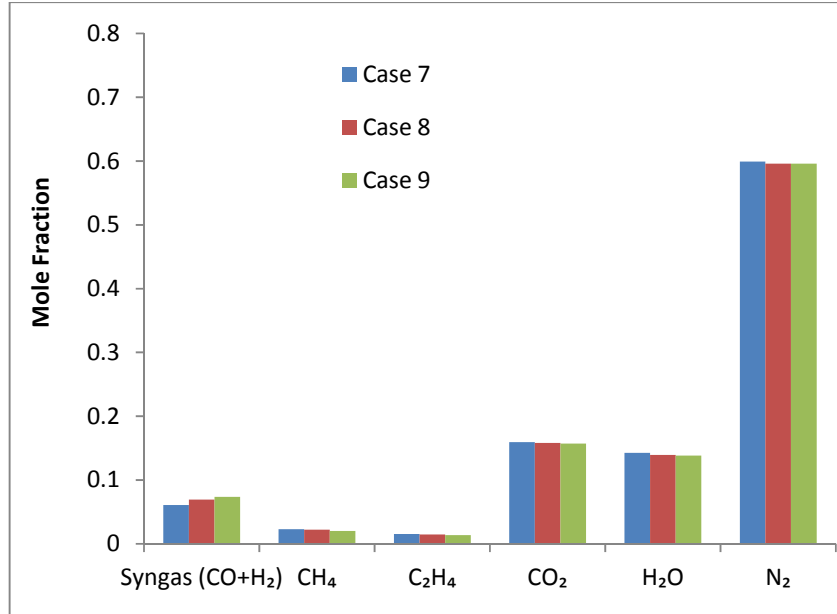


Figure 50: Outlet Gas Composition from Case 7-9

Figure 51 demonstrates the temperature profiles from cases 4-6, and the peak temperature predicted from case 4 appears earlier than those of cases 5 and 6. As mentioned in Section 4.4.2, it may be caused by faster gas combustion. Accordingly, O₂ composition in Case 4 then decreases more quickly than those of Cases 5 and 6, as displayed in Figure 52.

Figures 53-55 show the distributions of CH₄, C₂H₄, and syngas for cases 4-6. As displayed in the figures, the gas composition distributions from cases 4-6 follow the trends analogous to those of cases 1-3. According to our model, similar results of temperature and gas composition comparisons are also found in cases 7-9. Thus, the impacts of θ on the temperature and gas composition profiles discovered in Sections 4.4.2 and 4.4.3 are again confirmed with the comparison results from other cases by increasing air supply to the gasifier.

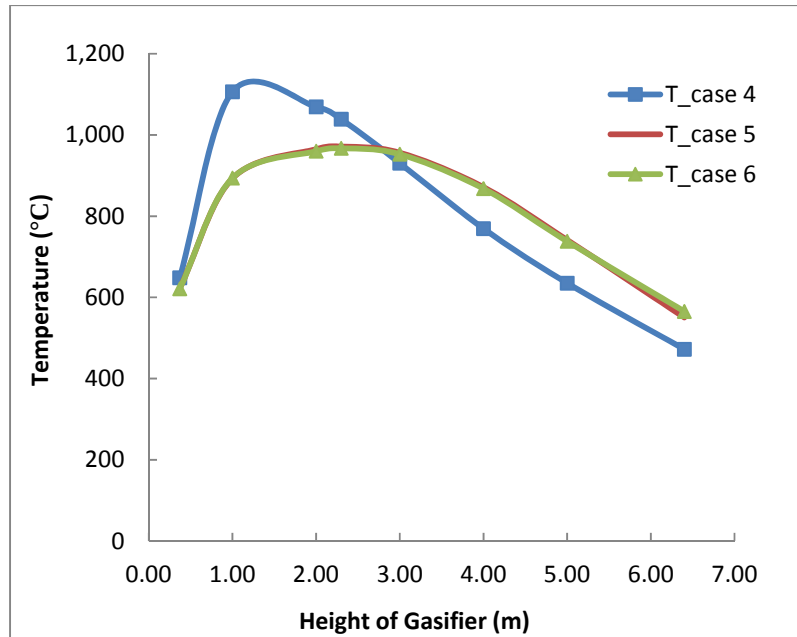


Figure 51: Temperature Profiles from Cases 4-6

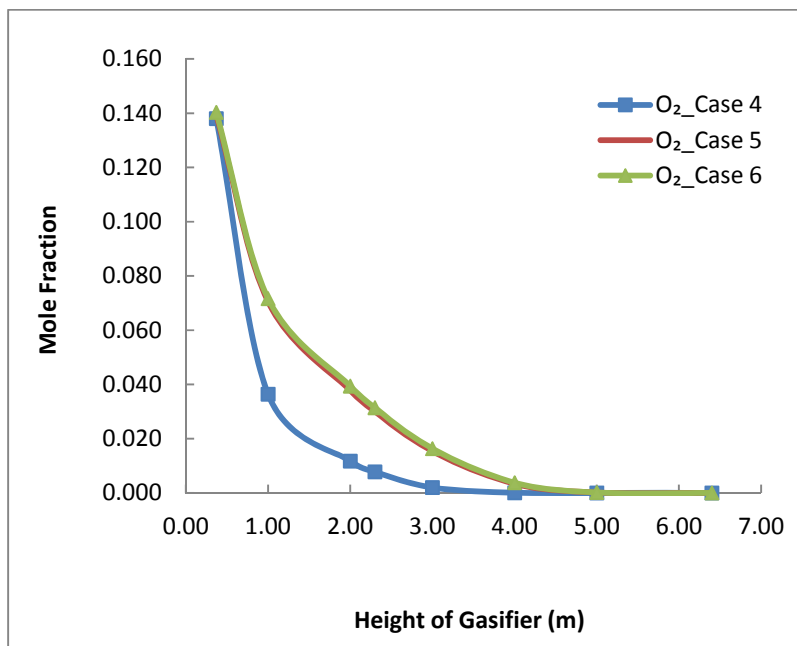


Figure 52: O₂ Distribution inside the Gasifier (Cases 4-6)

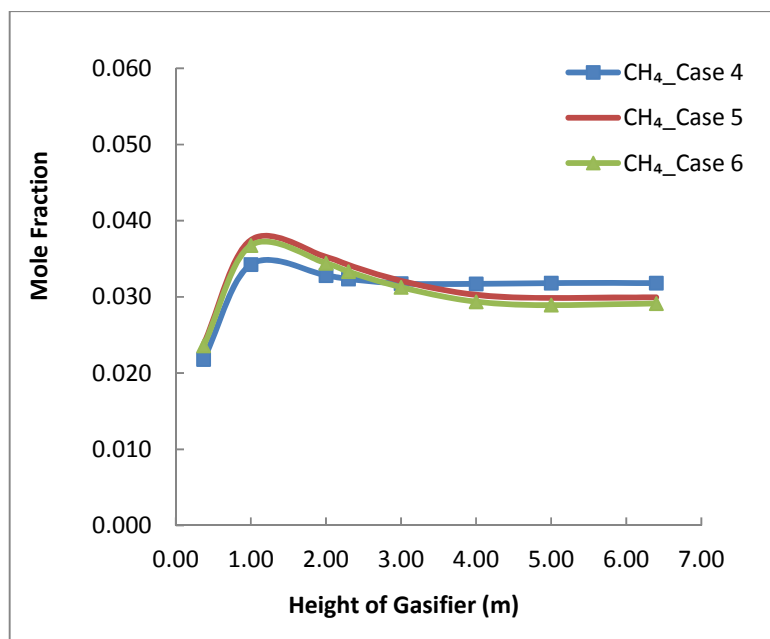


Figure 53: CH₄ Distribution inside the Gasifier (Cases 4-6)

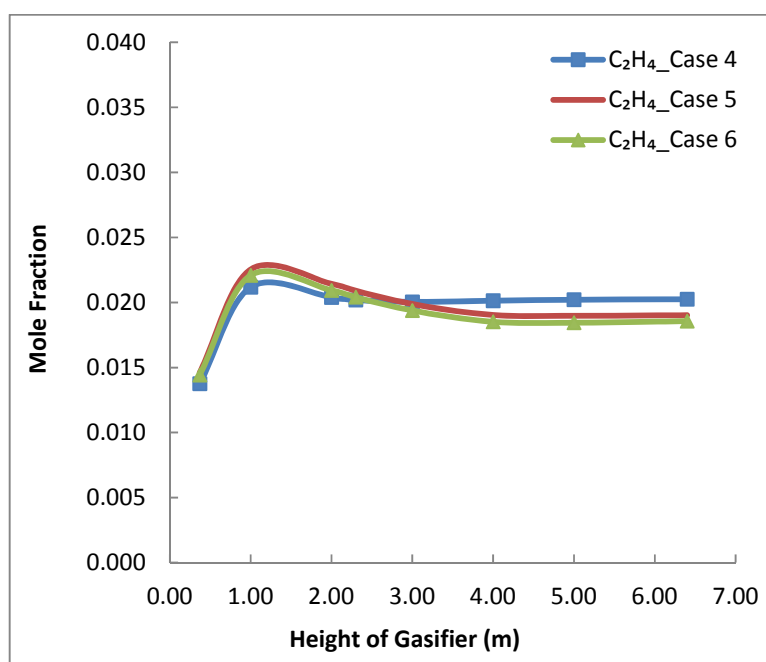


Figure 54: C₂H₄ Distribution inside the Gasifier (Cases 4-6)

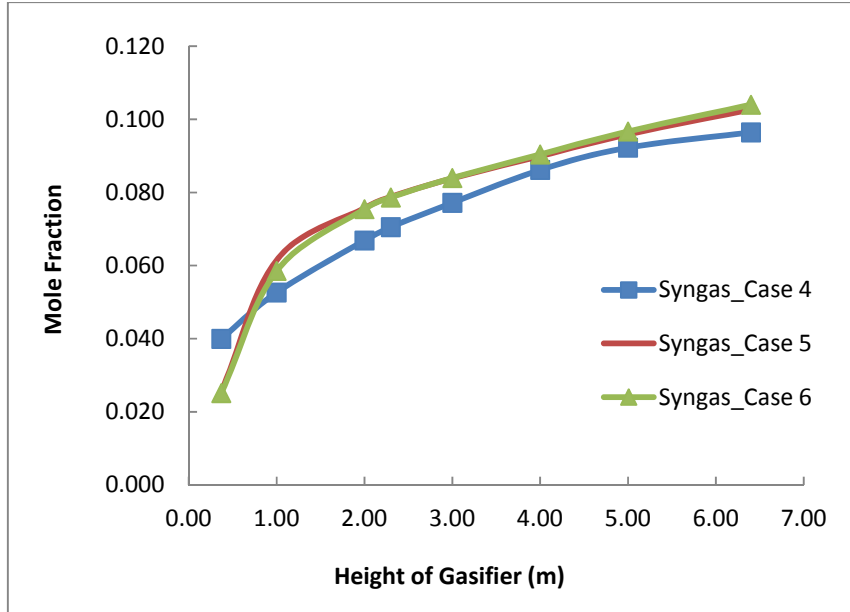


Figure 55: Syngas Distribution inside the Gasifier (Cases 4-6)

Figures 56-58 show the profiles of CH_4 , C_2H_4 , and syngas, respectively, for cases 1, 4, and 7. As seen in the figures, for the cases using the same value of θ , the mole fractions of CH_4 , C_2H_4 , and syngas decrease when the air flow rate increases from 109 to 147 Nm^3/h . It is mainly because when more air or O_2 is supplied to the gasifier, more combustible gases such as CH_4 , C_2H_4 , and syngas will react with O_2 . As a result of more gas combustion, the gasifier temperature also rises up, whilst the air flow rate increases, as shown in Figure 59.

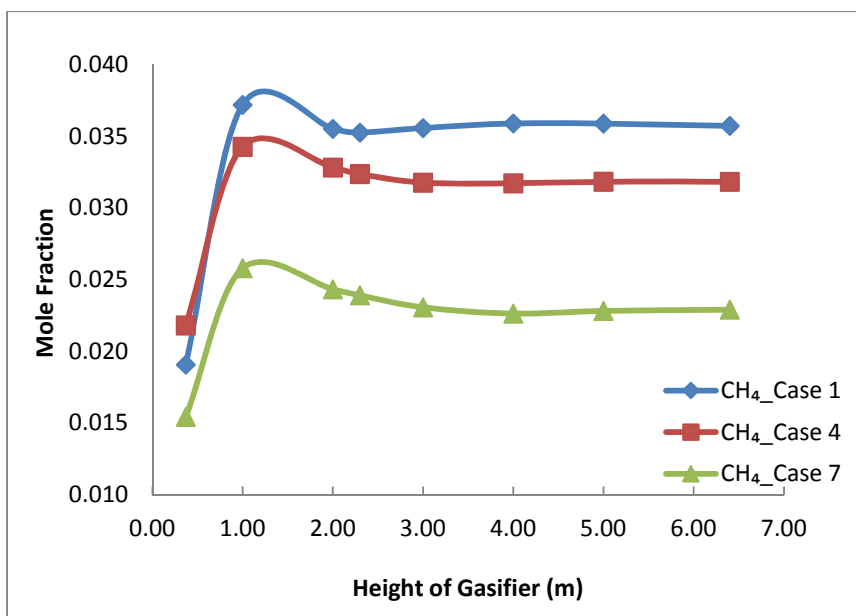


Figure 56: Comparison of CH₄ Distributions from Cases 1, 4, and 7

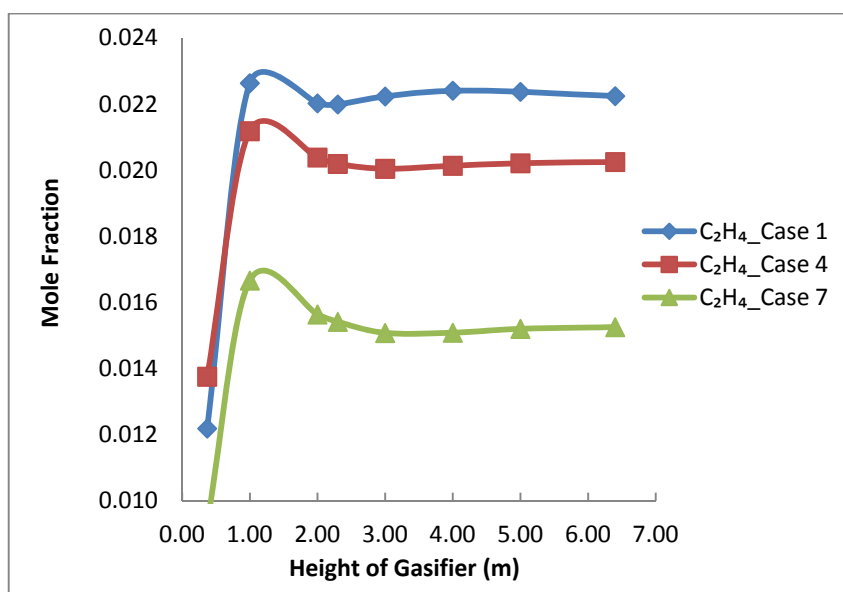


Figure 57: Comparison of C₂H₄ Distributions from Cases 1, 4, and 7

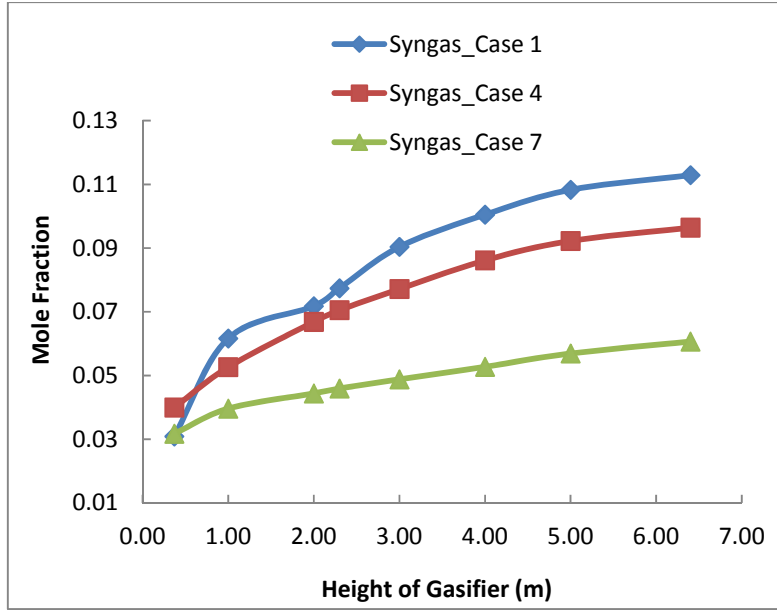


Figure 58: Comparison of Syngas Distributions from Cases 1, 4, and 7

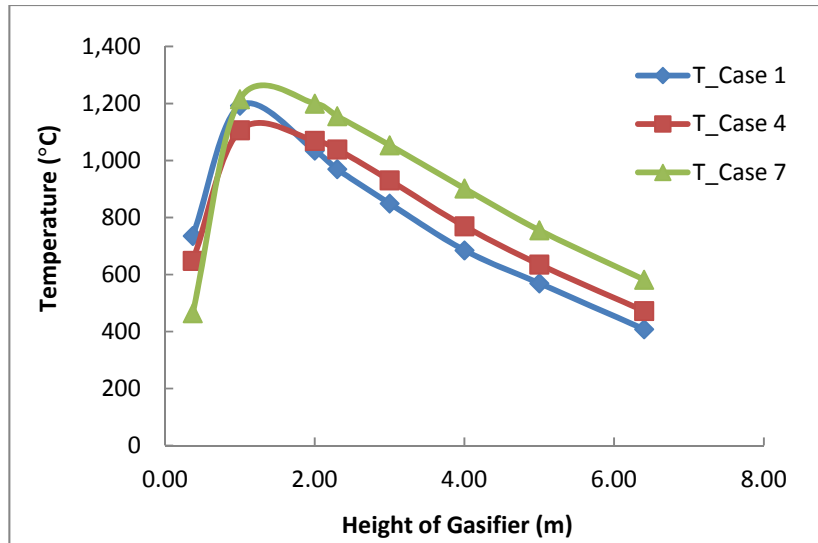


Figure 59: Comparison of Temperature Profiles from Cases 1, 4, and 7

4.5 Conclusions

In this paper, a 3D unsteady-state model was built to simulate biomass gasification using a CFB reactor. The RNG k-epsilon turbulence model was coupled with the enhanced wall treatment to describe turbulent flows in the gasifier. The equations of mass, momentum,

and energy conservation were applied to model mass and energy transfer in the reactor. The simulation results were compared and validated with experimental data. Nine cases were set up to examine the effect of θ , product distribution coefficient of char combustion.

According to the comparison of outlet gas compositions from the cases, the coefficient of θ showed a little impact on the prediction of outlet gas composition. It might be because except char combustion, other chemical reactions such as pyrolysis, and char gasification reactions also play major roles in producing gases. On the other hand, it was found that θ could affect the gasifier temperature profile. The reactor temperature from the cases with the value of 0.50 for θ increased more quickly than those in the cases using the values of 0.75 and 1.0, due to higher rates of gas combustion. It was also observed that the peak-temperature region or combustion zone moved to a higher region of the gasifier when the air supply to the gasifier increased.

Chapter 5

Conclusions and Recommendations

5.1 Conclusions

In Chapter 2, a 2-D unsteady-state hydrodynamic model was first established to investigate the impacts of standard wall function and drag models. The fluctuating energy equation was applied to describe the granular flow in a CFB riser, and the standard k-epsilon turbulence model was integrated with the standard wall function to describe the turbulent flow in the riser.

The simulation results were validated by the experimental data [40, 41]. A grid study was implemented to investigate the impact of the standard wall function. It was found that the standard wall functions played a major role in predicting the profile of solid volume fraction in the near-wall region, and the validity of the standard wall function could be greatly affected by the value of y^* . The value of y^* , in the range of 11.225 to 300, was preferable for the current hydrodynamic model.

The effects of the conventional and EMMS drag models were examined as well. The EMMS drag model showed less universal than the conventional drag models. In order to correctly describe the radial profile of solid volume fraction, the parameter settings of EMMS model might need to vary from case to case. However, the EMMS model also showed some advantages over the conventional drag models and was capable of presenting a temporal-varying profile and demonstrating three distinct solid regions in the riser.

In Chapter 3, the continuity, momentum, mass species reactions were integrated with the kinetics of heterogeneous char reaction and homogeneous gas-phase reactions to simulate biomass gasification in a CFB reactor. The effect of turbulence models was examined, and it was found that the difference between the standard k-epsilon, RNG, and the realizable k-epsilon models were insignificant. Meanwhile, it was also observed that the impact of thermal radiation is significant on the predictions of gasifier temperature

profiles, and the effect of thermal cannot be ignored. The role of WGS reaction was investigated in the study as well, and it was concluded that the kinetics of WGS reaction needed to be applied cautiously to the modeling of CFB biomass gasification, due to the non-catalytic environment and short reactor residence time of the CFB gasifier.

In Chapter 4, a 3-D unsteady-state CFD model was established to study the impact of char combustion production distribution coefficient. Three different values, 0.5, 0.75, and 1.0 were assigned to θ , and nine cases were built to examine the effect of this coefficient. According to the comparison, the coefficient, θ , showed minor impact on the predictions of outlet gas compositions; however, it was also seen that the coefficient could affect the prediction of gasifier temperature, and the high temperature area appeared earlier for the cases with $\theta=0.5$ than those of other cases. The similar impact of θ was also confirmed in other case studies where various air flow rate or ER were applied. Additionally, it was observed that the compositions of combustible gas species such as CH_4 , C_2H_4 , and syngas decreased and the gasifier temperature increased when the air flow rate or ER increased.

5.2 Recommendations for Future Work

As shown in the thesis, the CFD modeling of biomass gasification can present more comprehensive view than other conventional modeling techniques, and the profiles of velocity, temperature, and gas composition can be valuable for gasifier process design and optimization. The following are the recommendations for future investigation:

- For the hydrodynamic study, 3-D unsteady-state hydrodynamic models coupled with the conventional or EMMS drag models can present more details of turbulent flow in the riser than 2-D models. Accordingly, the transverse profiles of velocity and solid volume fraction can then be seen and compared with each other, which may help to obtain deeper understanding of the hydrodynamics of CFB gasifier.
- For the simulation of CFB gasification, two-step or multi-step reaction mechanism can be applied to the kinetics of biomass pyrolysis to present more details of CFB gasifier.

- Considering the limitations of Eulerian-Eulerian approach, the Eulerian-Lagrangian can be applied in future study to present more accurate predictions of velocity, temperature, and gas composition.
- Furthermore, instead of the Reynolds-averaged Navier-Stokes (RANS) turbulence models used in this work, the Large Eddy Simulation (LES) method can also be applied to the gas phase to further increase the accuracy of CFD model, as indicated by Chen and Ghoniem [119].

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Appendix A: Types of Gasifiers

A.1 Moving Bed/Fixed Bed Gasifier

“Moving bed” refers to as the “moving” fuel particles injected from the top of a gasifier, while “Fixed Bed” refers to as the fixed shape of bed where carbonaceous particles react with gasifying agents. Moving bed/fixed bed gasifiers consist of updraft, downdraft, and cross-draft gasifiers.

A.1.1 Updraft Gasifier

Figure A1 displays an updraft gasifier. In such a gasifier, the carbonaceous particles are fed from the top, descend and encounter the air blowing from the distributor at the bottom. The product gases are extracted from the outlet at the side of the gasifier, whilst the ash is collected and removed from the bottom [120, 121].

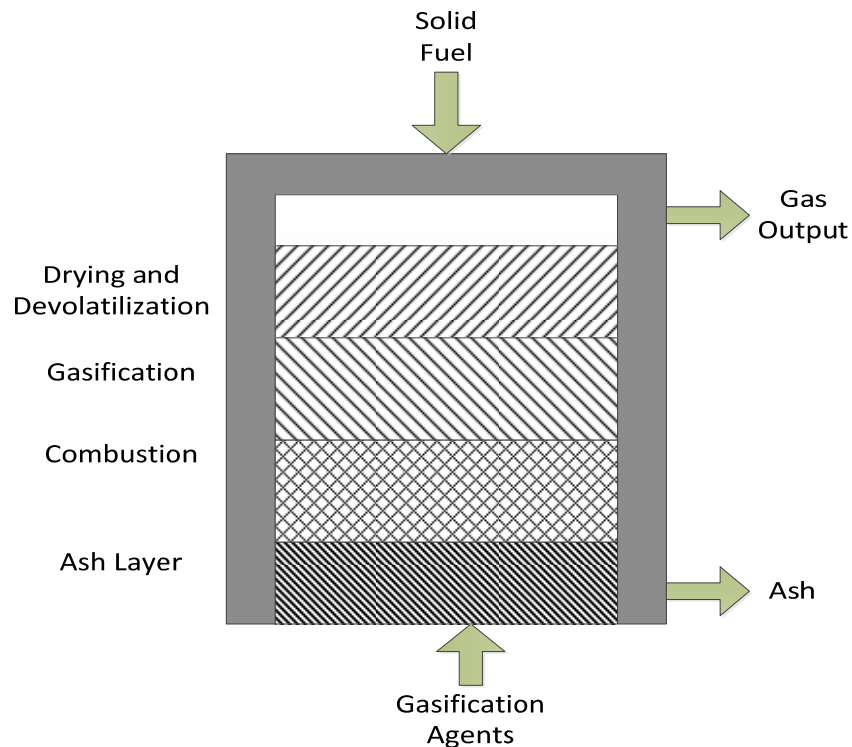


Figure A 1: Schematic of Updraft Gasifier

In this countercurrent flow system, the descending carbonaceous particles undergo drying, devolatilization, pyrolysis, char gasification and combustion process sequentially. Since the gas stream exits right after travelling through the zone of drying and pyrolysis, some parts of volatiles from the pyrolysis can be entrained outside the gasifier. Therefore, the tar content generated in an updraft gasifier is much higher than other gasifiers. Thus, an updraft moving bed gasifier may not be preferable for high-volatile fuels.

A.1.2 Downdraft Gasifier

As demonstrated in Figure A2, downdraft gasifier is a concurrent flow unit where both the carbonaceous particles and the gas stream flow in the same direction.

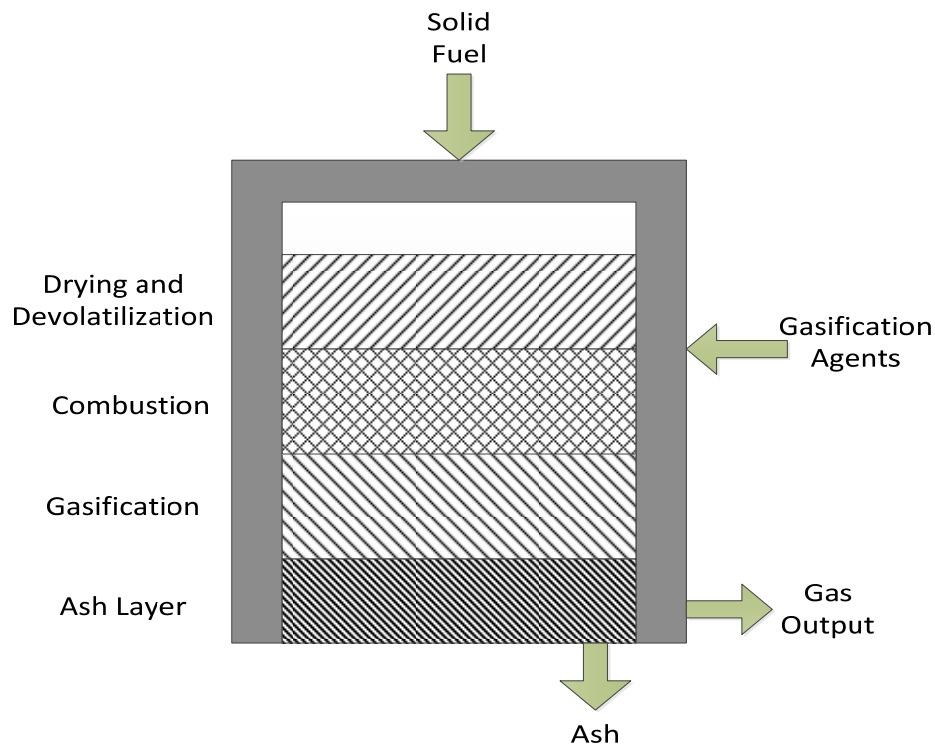


Figure A 2: Schematic of Downdraft Gasifier

Since air enters from the side, flows downward, and exits at the bottom, the volatiles generated during pyrolysis are forced to travel through the zones of combustion and gasification at above 900 °C, and the tar can be cracked into the non-condensable gases like carbon monoxide, carbon dioxide and other gases. As a result, the tar content in a downdraft gasifier is lower than an updraft gasifier.

A.1.3 Crossdraft Gasifier

In a crossdraft gasifier, as shown in Figure A3, biomass or fuel particles are fed from the top while air is injected from the side. The product gases exit at the other side of the gasifier, which is different from a downdraft gasifier where the product gases exit at the bottom.

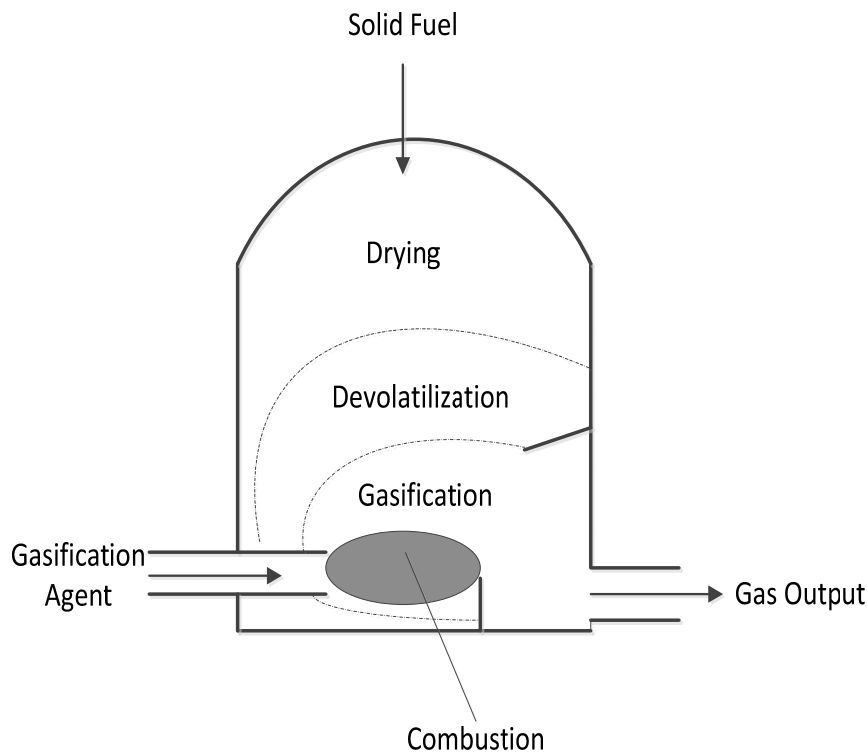


Figure A 3: Schematic of Crossdraft Gasifier

Crossdraft gasifiers are usually applied for small scale production, thus, the size of gasifier is generally small. On the other hand, the reactions may begin quickly due to the small reaction zone.

A.2 Fluidized Bed Gasifier

Figure A4 shows the schematic diagram of fluidized bed gasifier. In fluidized bed gasifiers, a better mixing of carbonaceous solid particles and gasifying agents can be

achieved when the particles are fluidized by the gasifying agents. As a result, mass and energy transfer in such a gasifier is also better than the ones in a fixed/moved bed gasifier.

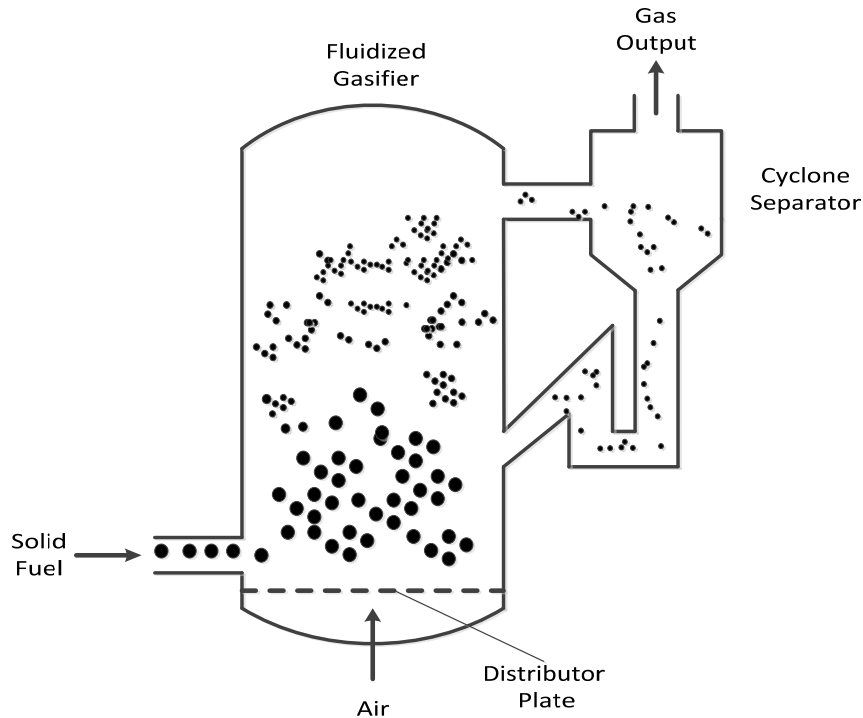


Figure A 4: Schematic Diagram of Fluidized Bed Gasifier

A.2.1 Bubbling Fluidized Bed Gasifier

In a bubbling fluidized bed gasifier, the carbonaceous solid fuel, generally crushed into less than 10 mm particles, is fed into the gasifier and is fluidized by the gasifying mediums delivered from the bottom. Some bubbles appear when the gas travels through the bed. A small amount of particles are lifted up in the space (freeboard), and then most of them will fall back to the bed. Some light particles (dusts) are taken outside the gasifier. They are captured in a cyclone and then returned to the gasifier.

In addition to the gasifying mediums supplied from the bottom, a supplementary gasifying medium can be introduced from the lower side of the gasifier. The purpose of that is to react with the un-reacted char particles remained in the freeboard space (the space above the bed) to achieve a higher conversion of carbonaceous fuel.

The flow regime in a bubbling fluidized bed presents much better mixing of gas and particles than fixed bed gasifiers. Such a gasifier is suitable for medium scale production [122, 123].

A.2.2 Circulating Fluidized Bed Gasifier

A circulating fluidized bed gasifier typically includes a riser serving as a reactor, an external recycle cyclone, and a seal pot.

Since the gas velocity in a CFB gasifier, generally 3.5-5 m/s, is higher than bubbling fluidized bed, 0.5-1.0 m/s, the hydrodynamics in such a gasifier is also different from bubbling fluidized bed gasifiers. Unlike a bubbling fluidized bed gasifier where the particles mostly remain in the bed, all of the particles in a CFB riser (circulating fluidized bed) are lifted up and mixed with the gases thoroughly due to turbulence flow situation and strong dragging force caused by high slip velocity between the particles and gases. So, in a CFB gasifier, a better mixing between gas and particles can be achieved and as a result it also provides more efficient mass and energy transfer for gasification reactions [124-126].

A.3 Entrained Flow Gasifier

Entrained flow gasifiers are essentially concurrent reactors. Very fine carbonaceous solid particles, generally coal particles, combined with gasifying mediums are injected into the gasifier from the top or side. Gasification reactions occur above 1000 °C within a few seconds.

Figure A5 demonstrates the schematic diagram of entrained flow gasifier, where fuel particles are injected into the gasifier from the top together with gasifying agents such as oxygen gas and steam.

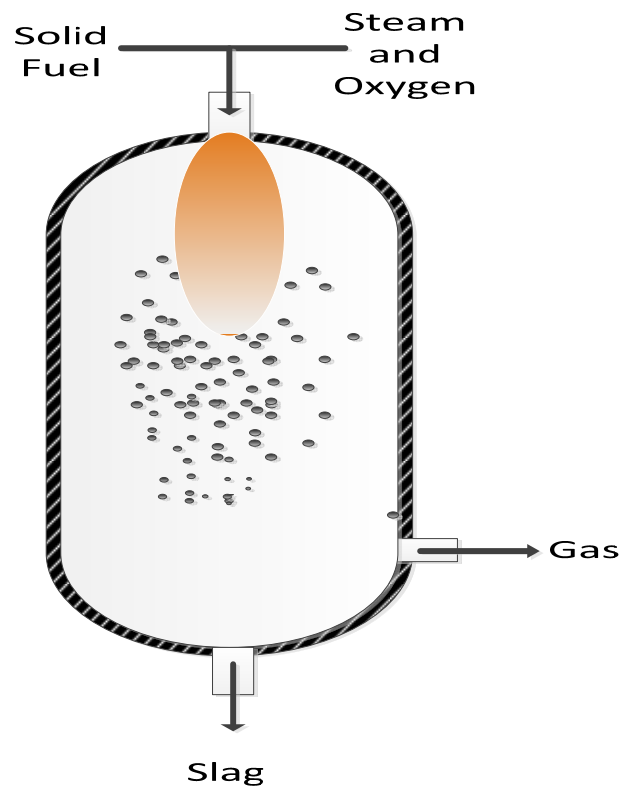


Figure A 5: Schematic Diagram of Entrained Flow Gasifier

Appendix B: Standard k-epsilon Turbulence Model, Kinetic Theory of Granular Flow, and Energy Transport Equation

B.1 Standard k-epsilon Turbulence Model

The velocity in turbulent flow fluctuates in a chaotic fashion and cannot be solved directly from the “Navier-Stokes Equations”. Therefore, proper models are needed to describe turbulent flows [127]. A technique used in the derivation of turbulent flow modeling is Reynolds-averaged technique that partitions instantaneous velocity into mean velocity and fluctuating component in the following form [128]:

$$u_i = u'_i + \bar{u}_i \quad (\text{B-1})$$

where u_i is the instantaneous velocity, u'_i is the fluctuating velocity, and $\bar{u}_i$ is the mean velocity.

The Navier-Stokes Equation is given by

$$\rho \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \rho g_i - \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_i} \quad (\text{B-2})$$

where i, j are the coordinates.

Taking the Reynolds-averaged technique, the equation above becomes as follows:

$$\overline{\rho \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}} = \overline{\rho g_i - \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_i}} \quad (\text{B-3})$$

or

$$\rho \overline{\frac{\partial u_i}{\partial t}} + \overline{\rho u_j \frac{\partial u_i}{\partial x_j}} = \overline{\rho g_i} - \overline{\frac{\partial p}{\partial x_i}} - \overline{\frac{\partial \tau_{ij}}{\partial x_i}} \quad (\text{B-4})$$

Substitute Equation B-1 into the second term on the left side of Equation B-4,

$$\begin{aligned} \overline{u_j \frac{\partial u_i}{\partial x_j}} &= \overline{(\bar{u}_j + u'_j) \frac{\partial (\bar{u}_i + u'_i)}{\partial x_j}} \\ &= \overline{\bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\bar{u}_j \frac{\partial u'_i}{\partial x_j}} + \overline{u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{u'_j \frac{\partial u'_i}{\partial x_j}} \\ &= \overline{\bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\bar{u}_j \frac{\partial u'_i}{\partial x_j}} + \overline{u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{u'_j \frac{\partial u'_i}{\partial x_j}} \end{aligned}$$

$$= \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} + \overline{u_j} \frac{\partial \overline{u'_i}}{\partial x_j} + \overline{u'_j} \frac{\partial \overline{u_i}}{\partial x_j} + \overline{u'_j} \frac{\partial \overline{u'_i}}{\partial x_j} \quad (\text{B-5})$$

According to the definition of fluctuating velocity[127], $\frac{\partial \overline{u'_i}}{\partial x_j}$ and $\overline{u'_i}$ are zero, thus the equation becomes:

$$\overline{u_j \frac{\partial u_i}{\partial x_j}} = \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} + \overline{u'_j} \frac{\partial \overline{u'_i}}{\partial x_j} \quad (\text{B-6})$$

where $\overline{u'_j \frac{\partial u'_i}{\partial x_j}}$ can be calculated by the equations below,

$$\overline{u'_j \frac{\partial u'_i}{\partial x_j}} = \frac{\partial \overline{u'_j u'_i}}{\partial x_j} - \overline{u'_i} \frac{\partial \overline{u'_j}}{\partial x_j} \quad (\text{B-7})$$

and

$$\begin{aligned} \overline{u'_1 \frac{\partial u'_1}{\partial x_1} + u'_1 \frac{\partial u'_2}{\partial x_2} + u'_1 \frac{\partial u'_3}{\partial x_3}} & \quad i = 1, j = 1, 2, 3 \\ \overline{u'_i \frac{\partial u'_j}{\partial x_j}} &= \overline{u'_2 \frac{\partial u'_1}{\partial x_1} + u'_2 \frac{\partial u'_2}{\partial x_2} + u'_2 \frac{\partial u'_3}{\partial x_3}} \quad i = 2, j = 1, 2, 3 \\ \overline{u'_3 \frac{\partial u'_1}{\partial x_1} + u'_3 \frac{\partial u'_2}{\partial x_2} + u'_3 \frac{\partial u'_3}{\partial x_3}} & \quad i = 3, j = 1, 2, 3 \end{aligned} \quad (\text{B-8})$$

According to the continuity equation, the following equations are shown as follows:

$$\begin{aligned} \overline{u'_1 \left(\frac{\partial u'_1}{\partial x_1} + \frac{\partial u'_2}{\partial x_2} + \frac{\partial u'_3}{\partial x_3} \right)} &= 0 \quad i = 1, j = 1, 2, 3 \\ \overline{u'_2 \left(\frac{\partial u'_1}{\partial x_1} + \frac{\partial u'_2}{\partial x_2} + \frac{\partial u'_3}{\partial x_3} \right)} &= 0 \quad i = 2, j = 1, 2, 3 \\ \overline{u'_3 \left(\frac{\partial u'_1}{\partial x_1} + \frac{\partial u'_2}{\partial x_2} + \frac{\partial u'_3}{\partial x_3} \right)} &= 0 \quad i = 3, j = 1, 2, 3 \end{aligned} \quad (\text{B-9})$$

Substituting Equation B-9 and B-8 into B-7, Equation B-10 is obtained:

$$\overline{u'_j \frac{\partial u'_i}{\partial x_j}} = \frac{\partial \overline{u'_j u'_i}}{\partial x_j} \quad (\text{B-10})$$

Thus, substituting Equation B-6 and Equation B-10 into Equation B-4 and re-arranging the equation, the turbulent momentum equation is derived as follows:

$$\rho \frac{\partial \overline{u_i}}{\partial t} + \rho \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} = \rho g_i - \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \overline{\tau_{ij}}}{\partial x_i} - \frac{\partial \overline{\rho u'_j u'_i}}{\partial x_j} \quad (\text{B-11})$$

Defining $\overline{\rho u'_j u'_i}$ as τ_{ij}^t , turbulent Reynolds stress tensor, thus the turbulent equation can be stated as:

$$\rho \frac{\partial \overline{u_i}}{\partial t} + \rho \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} = \rho g_i - \frac{\partial \overline{p}}{\partial x_i} - \left(\frac{\partial \overline{\tau_{ij}}}{\partial x_i} + \frac{\partial \tau_{ij}^t}{\partial x_i} \right) \quad (\text{B-12})$$

The momentum equation above is not in a closed form yet because the term $\overline{\rho u'_j u'_i}$ or τ_{ij}^t is still unknown. So, a turbulent stress tensor model analogous to the laminar viscous tensor has been defined [39]:

$$\tau_{ij}^t = -\mu_t \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} - \frac{2}{3} \overline{\nabla \cdot \vec{v}} \delta_{ij} \right) + \frac{2}{3} \rho k \delta_{ij} \quad (\text{B-13})$$

δ_{ij} (Kronecker Delta, a unit tensor) = 1, $i = j$,

δ_{ij} (Kronecker Delta, a unit tensor) = 0, $i \neq j$.

$$\mu_t = \frac{\rho C_\mu k^2}{\varepsilon} \quad (\text{B-14})$$

where k is turbulent kinetic energy, defined as $\frac{\overline{u'_i u'_i}}{2}$,

ε is turbulent kinetic energy dissipation rate, defined as $\mu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j}$,

C_μ is a turbulent modeling constant.

Comparatively, the laminar viscous tensor is shown below,

$$\tau_{ij} = -\mu \left[\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) - \left(\frac{2}{3} \overline{\nabla \cdot \vec{u}} \delta_{ij} \right) \right] \quad (\text{B-15})$$

where μ is laminar viscosity.

As shown above, in order to solve turbulent momentum equation B-12, k and ε must be modeled. The widely accepted $k - \varepsilon$ and turbulent momentum equations were achieved and shown as follows [39]:

Turbulent Momentum Equation:

$$\rho \frac{\partial \overline{u_i}}{\partial t} + \rho \overline{u_j} \cdot \nabla \overline{u_i} = \rho \vec{g} - \nabla p + \nabla \cdot [(\mu + \mu_t) \left(\overline{\nabla \vec{u}} + \overline{\nabla \vec{u}^T} - \frac{2}{3} \overline{\nabla \cdot \vec{v}} \delta_{ij} \right)] - \frac{2}{3} \nabla(\rho k \delta_{ij}) \quad (\text{B-16})$$

Turbulent Kinetic Energy Equation:

$$\rho \frac{\partial k}{\partial t} + \rho \bar{\vec{u}} \cdot \nabla k = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + \mu_t p(\bar{\vec{u}}) - \frac{2\rho k}{3} \nabla \cdot \bar{\vec{u}} - \rho \varepsilon \quad (\text{B-17})$$

Turbulent Kinetic Energy Dissipation Rate Equation:

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \bar{\vec{u}} \cdot \nabla \varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \frac{C_{\varepsilon 1} \varepsilon}{k} \left[\mu_t p(\bar{\vec{u}}) - \frac{2\rho k}{3} \nabla \cdot \bar{\vec{u}} \right] - \frac{C_{\varepsilon 2} \rho \varepsilon^2}{k} \quad (\text{B-18})$$

where $p(\bar{\vec{u}}) = \nabla \bar{\vec{u}} : \left(\overline{\nabla \bar{\vec{u}}} + \overline{\nabla \bar{\vec{u}}^T} \right) - \frac{2}{3} (\nabla \cdot \bar{\vec{u}})^2$ and σ_k , σ_ε , $C_{\varepsilon 1}$, and $C_{\varepsilon 2}$ are modeling constants, usually 1.0, 1.3, 1.44 and 1.92, respectively [39].

B.2 Kinetic Theory of Granular Flow

The turbulent momentum (B-16), turbulent kinetic energy (B-17) and dissipation rate equations (B-18) can be applied to both gas and particle phases. However for the particle phase, particle phase viscosity, a very important parameter, is hardly measureable because it can vary significantly due to different diameters of particles, thus a model needs to be established to estimate this parameter.

Kinetic theory of granular flow, as a part of quantum mechanics, is to study particle motions at microscopic level and explain macroscopic phenomena. Based on a binary particle collision assumption, some parameters such as diffusivity and viscosity can be estimated quite accurately using this theory. Since kinetic theory of granular flow was originated from the well-known ‘‘Boltzmann-Maxwell Equation’’ [129].

B.2.1 Boltzmann-Maxwell Equation

The Boltzmann-Maxwell equation was first developed in the 1860s and 1870s by the physicists, James Clerk Maxwell and Ludwig Boltzmann, to predict the distribution of gaseous molecules and its relations with gas temperature, pressure and velocity. In recent years, a theory on particle or granular flow, known as kinetic theory of granular flow, has been developed from this equation, and it has been proved quite accurate for estimating some transport coefficients such as diffusivity and viscosity.

Velocity Distribution Function

As defined in Boltzmann-Maxwell Equation [130], some macroscopic properties can be estimated from the velocity distribution of molecules f , which is a function of time t , position r and instantaneous velocity c , shown as follows.

$$f = f(t, r, c) \quad (\text{B-19})$$

The hypothesis of this velocity distribution is that at time t , in the element dr , the number of molecules in a unit volume, n , is calculated by the following equations

$$n dr = \iint f dc dr \quad (B-20)$$

Thus, the following equation is achieved,

$$n = \int f dc \quad (B-21)$$

For a quantity ϕ , being a scalar or, vector or tensor, the sum of ϕ at time t and in the element dr , is defined as:

$$\begin{aligned} \Sigma \phi &= n \bar{\phi} dr \\ &= dr \int \phi f dc \end{aligned} \quad (B-22)$$

Therefore, the mean of the quantity ϕ is

$$n \bar{\phi} = \int \phi f dc \quad (B-23)$$

Let ϕ be the molecule instantaneous velocity, c , then the mean velocity v is

$$nv = \int cf dc \quad (B-24)$$

or

$$v = \frac{1}{n} \int cf dc \quad (B-25)$$

Boltzmann-Maxwell Equation

Boltzmann-Maxwell Equation is based on a hypothesis that during the time, dt . Each molecule is exerted a force F , then the velocity of molecule is $c + Fdt$, and the position vector becomes $r + cdt$. The function $f(c + Fdt, r + cdt, t + dt)$ is different from $f(c, r, t)$ due to a binary particle collision. Thus the following equation is obtained:

$$\{f(c + Fdt, r + cdt, t + dt) - f(c, r, t)\} dc dr = \left(\frac{\partial f}{\partial t}\right)_{coll} dc dr dt \quad (B-26)$$

Dividing both sides by $dc dr dt$ and taking dt close to zero, the following is obtained:

$$\frac{f(c+Fdt, r+cdt, t+dt) - f(c, r, t)}{dt} = \left(\frac{\partial f}{\partial t}\right)_{coll} \quad (B-27)$$

According to First Order Taylor Series Expansion, Equation B-27 can be approximated to:

$$\begin{aligned}
& \frac{f(c + Fdt, r + cdt, t + dt) - f(c, r, t)}{dt} \\
&= \frac{\left\{ f(c, r, t) + \frac{\partial f}{\partial c}(c + Fdt - c) + \frac{\partial f}{\partial r}(r + cdt - r) + \frac{\partial f}{\partial t}(t + tdt - t) \right\} - f(c, r, t)}{dt} \\
&= \frac{\frac{\partial f}{\partial c} \cdot Fdt + \frac{\partial f}{\partial r} \cdot cdt + \frac{\partial f}{\partial t} \cdot dt}{dt} \\
&= \frac{\partial f}{\partial t} + F \cdot \frac{\partial f}{\partial c} + c \cdot \frac{\partial f}{\partial r}
\end{aligned} \tag{B-28}$$

Thus Boltzmann-Maxwell Equation is achieved:

$$\frac{\partial f}{\partial t} + F \cdot \frac{\partial f}{\partial c} + c \cdot \frac{\partial f}{\partial r} = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{B-29}$$

Multiplying both sides by ϕ and integrating over dc , the following equation yields:

$$\int \phi \left(\frac{\partial f}{\partial t} + F \cdot \frac{\partial f}{\partial c} + c \cdot \frac{\partial f}{\partial r} \right) dc = \int \phi \left(\frac{\partial f}{\partial t} \right)_{coll} dc \tag{B-30}$$

$$\text{Define } c = \mathbf{C} + \mathbf{v} \tag{B-31}$$

where c , $\mathbf{C}$ and $\mathbf{v}$ are instantaneous velocity, fluctuating velocity and mean velocity, respectively.

Substituting Equation B-31 into B-30 and with further manipulation as done by Sydney and Cowling [130], the following equation is obtained:

$$\frac{Dn\bar{\phi}}{Dt} + n\bar{\phi}\nabla \cdot \mathbf{v} + \frac{\partial n\bar{\phi}\mathbf{C}}{\partial r} - n \left(F - \frac{Dv}{Dt} \right) \frac{\partial \bar{\phi}}{\partial c} - n \frac{\partial \bar{\phi}}{\partial c} \mathbf{C} : \frac{\partial \mathbf{v}}{\partial r} = n\bar{\phi}_{coll} \tag{B-32}$$

where $\frac{D}{Dt}$ is a “substantial derivative”, defined as follows:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \tag{B-33}$$

$\bar{\phi}_{coll}$ is the average change of the quantity caused by the particle collision and is defined as follows:

$$n\bar{\phi}_{coll} = -\nabla \cdot \mathbf{P}_{coll} + N_{coll} \tag{B-34}$$

$\mathbf{P}_{coll}$ is a function of $(\phi_1' - \phi_1)$ multiplied by other elements such as the unit vectors defined by the binary particle theory [32].

N_{coll} is a function of $(\phi_1' + \phi_2' - \phi_1 - \phi_2)$ multiplied by other elements such as the unit vectors defined by the binary particle theory [32].

$\phi_1, \phi_2, \phi_1', \phi_2'$ are the quantities ϕ of particle 1 and particle 2 before and after binary particle collision.

B.2.2 Continuity Equation for the Particle Phase

Let $\phi = m$, particle mass, then Equation B-32 becomes:

$$\frac{Dn\bar{m}}{Dt} + n\bar{m}\nabla \cdot v + \frac{\partial n\bar{m}\bar{C}}{\partial r} - n\left(F - \frac{Dv}{Dt}\right)\frac{\partial \bar{m}}{\partial C} - n\frac{\partial \bar{m}}{\partial C}\bar{C}:\frac{\partial v}{\partial r} = n\overline{\phi_{coll}(m)} \quad (B-35)$$

In the equation above,

$nm = \rho$, and

$\frac{\partial n\bar{m}\bar{C}}{\partial r} = \frac{\partial nm\bar{C}}{\partial r} = 0$, because the mean of fluctuating velocity is defined as zero,

$\frac{\partial \bar{m}}{\partial C} = 0$,

$n\phi_{coll}(m) = 0$, because $(m_1' - m_1)$ and $(m_1' + m_2' - m_1 - m_2)$ are all zero according to the mass conservation law.

Thus the following equation is achieved:

$$\frac{Dnm}{Dt} + nm\nabla \cdot v = \frac{\partial \rho}{\partial t} + v \cdot \frac{\partial \rho}{\partial r} + \rho\nabla \cdot v = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (B-36)$$

B.2.3 Momentum Equation for the Particle Phase

Substituting $\phi = m\bar{C}$ into Equation B-32, then the following equation is achieved:

$$\frac{Dn\bar{m}\bar{C}}{Dt} + n\bar{m}\bar{C}\nabla \cdot v + \frac{\partial n\bar{m}\bar{C}\bar{C}}{\partial r} - n\left(F - \frac{Dv}{Dt}\right)\frac{\partial \bar{m}\bar{C}}{\partial C} - n\frac{\partial \bar{m}\bar{C}}{\partial C}\bar{C}:\frac{\partial v}{\partial r} = n\overline{\phi_{coll}(m\bar{C})} \quad (B-37)$$

The left Side

$$= \frac{Dn\bar{m}\bar{C}}{Dt} + n\bar{m}\bar{C}\nabla \cdot v + \frac{\partial n\bar{m}\bar{C}\bar{C}}{\partial r} - n\left(F - \frac{Dv}{Dt}\right)\left(\bar{C}\frac{\partial \bar{m}}{\partial C} + \bar{m}\frac{\partial \bar{C}}{\partial C}\right) - n\left(\bar{C}\frac{\partial \bar{m}}{\partial C} + \bar{m}\frac{\partial \bar{C}}{\partial C}\right)\bar{C}:\frac{\partial v}{\partial r}$$

Since $\bar{C} = 0$, the first two terms disappear. $\frac{\partial \bar{m}}{\partial C}$ is equal to zero, because the mass of particle is independent of the fluctuating velocity.

Therefore, the left side

$$\begin{aligned}
&= \frac{\partial nm\overline{CC}}{\partial r} - nm \left(F - \frac{Dv}{Dt} \right) - nm\overline{C}: \frac{\partial v}{\partial r} \\
&= \frac{\partial \rho\overline{CC}}{\partial r} - \rho \left(F - \frac{Dv}{Dt} \right)
\end{aligned}$$

Thus Equation B-37 becomes as follows:

$$\frac{\partial \rho\overline{CC}}{\partial r} - \rho \left(F - \frac{Dv}{Dt} \right) = \overline{n\phi(m\mathbf{C})_{coll}} \quad (\text{B-38})$$

Recall Equation B-34

$$n\overline{\phi}_{coll} = -\nabla \cdot P_{coll} + N_{coll}$$

And $N_{coll} = 0$ because $(m_1'\mathbf{C}_1' + m_2'\mathbf{C}_2' - m_1\mathbf{C}_1 - m_2\mathbf{C}_2) = 0$, according to the momentum conservation law, then

$$\overline{n\phi_{coll}(m\mathbf{C})} = -\nabla \cdot P_{coll}(m\mathbf{C}) \quad (\text{B-39})$$

Defining $\rho\overline{CC} = P_k$, the equation of particle momentum is achieved as:

$$\frac{\partial \rho\overline{CC}}{\partial r} - \rho \left(F - \frac{Dv}{Dt} \right) = -\frac{\partial(P_{coll}(m\mathbf{C}))}{\partial r}$$

or

$$\begin{aligned}
\left(\rho \frac{Dv}{Dt} \right) &= - \left(\frac{\partial(P_{coll}(m\mathbf{C}))}{\partial r} + \frac{\partial P_k}{\partial r} \right) + \rho F \\
&= -\nabla \cdot (P_{coll} + P_k) + \rho F
\end{aligned} \quad (\text{B-40})$$

For multiphase flows, the density mentioned in the momentum equations above is referred to as the bulk density and is defined in the following equation.

$$\rho = \rho_s \times \alpha_s \quad (\text{B-41})$$

where ρ and ρ_s are bulk density of particle phase and density of a particle, respectively, and α_s is volume fraction of particle phase.

In multiphase flows, the forces exerted on a particle include not only the gravity but also the drag force, and are defined as follows,

$$\rho F = \rho_s \alpha_s F = \alpha_s \rho_s g + \beta(v_g - v_s) \quad (\text{B-42})$$

Substituting Equation B-41 and Equation B-42 into Equation B-40, the following equation is obtained:

$$\left(\alpha_s \rho_s \frac{Dv}{Dt} \right) = \alpha_s \rho_s g - \nabla \cdot (P_{coll} + P_k) + \beta(v_g - v_s) \quad (\text{B-43})$$

Let $\tau_s = -(P_{coll} + P_k)$, which is total stress tensor of particle phase, then,

$$\left(\alpha_s \rho_s \frac{Dv}{Dt}\right) = \alpha_s \rho_s g + \nabla \cdot \tau_s + \beta(v_g - v_s) \quad (\text{B-44})$$

B.2.4 Fluctuating Kinetic Energy Equation for the Particle Phase

For Equation B-32, if one sets $\phi = \frac{1}{2} m \mathcal{C}^2$, it becomes as follows:

$$\begin{aligned} & \frac{Dn(\frac{1}{2}m\mathcal{C}^2)}{Dt} + n(\frac{1}{2}m\mathcal{C}^2)\nabla \cdot v + \frac{\partial n(\frac{1}{2}m\mathcal{C}^2)\mathcal{C}}{\partial r} - n\left(F - \frac{Dv}{Dt}\right)\frac{\partial(\frac{1}{2}m\mathcal{C}^2)}{\partial \mathcal{C}} - n\frac{\partial(\frac{1}{2}m\mathcal{C}^2)}{\partial \mathcal{C}}\mathcal{C}:\frac{\partial v}{\partial r} = \\ & n\phi(\frac{1}{2}m\mathcal{C}^2)_{coll} \end{aligned} \quad (\text{B-45})$$

Equation B-45 is substituted term by term. Define $\frac{1}{3}\overline{\mathcal{C}^2}$ as the granular temperature Θ , then

$$\frac{Dn(\frac{1}{2}m\mathcal{C}^2)}{Dt} = \frac{3}{2} \frac{Dnm\Theta}{Dt} = \frac{3}{2} \frac{D\rho\Theta}{Dt} \quad (\text{B-46})$$

$$n(\frac{1}{2}m\mathcal{C}^2)\nabla \cdot v = \frac{3}{2}nm\Theta\frac{\partial v}{\partial r} = \frac{3}{2}\rho\Theta\frac{\partial v}{\partial r}\nabla \cdot v \quad (\text{B-47})$$

Let $nm(\frac{1}{2}\mathcal{C}^2)\mathcal{C}$ or $\rho(\frac{1}{2}\mathcal{C}^2)\mathcal{C}$ be q_k , then

$$\begin{aligned} \frac{\partial n(\frac{1}{2}m\mathcal{C}^2)\mathcal{C}}{\partial r} &= \frac{\partial nm(\frac{1}{2}\mathcal{C}^2)\mathcal{C}}{\partial r} \\ &= \frac{\partial q_k}{\partial r} \end{aligned} \quad (\text{B-48})$$

$$\begin{aligned} -n\left(F - \frac{Dv}{Dt}\right)\frac{\partial(\frac{1}{2}m\mathcal{C}^2)}{\partial \mathcal{C}} &= -\left(F - \frac{Dv}{Dt}\right)\frac{1}{2}n\left(\frac{\partial m}{\partial \mathcal{C}} + m\frac{\partial \mathcal{C}^2}{\partial \mathcal{C}}\right) \\ &= -\left(F - \frac{Dv}{Dt}\right)\frac{1}{2}n\left(\frac{\partial m}{\partial \mathcal{C}}\mathcal{C}^2 + m2\mathcal{C}\right) \\ &= -\left(F - \frac{Dv}{Dt}\right)nm\bar{\mathcal{C}} = 0 \end{aligned} \quad (\text{B-49})$$

$$\begin{aligned} n\frac{\partial(\frac{1}{2}m\mathcal{C}^2)}{\partial \mathcal{C}}\mathcal{C}:\frac{\partial v}{\partial r} &= n\left(\frac{1}{2}\frac{\partial m}{\partial \mathcal{C}}\mathcal{C}^2 + \frac{1}{2}m\frac{\partial \mathcal{C}^2}{\partial \mathcal{C}}\right)\mathcal{C}:\frac{\partial v}{\partial r} \\ &= n\left(\frac{1}{2}\frac{\partial m}{\partial \mathcal{C}}\mathcal{C}^2 + m\mathcal{C}\right)\mathcal{C}:\frac{\partial v}{\partial r} \\ &= nm\bar{\mathcal{C}}\mathcal{C}:\frac{\partial v}{\partial r} \end{aligned}$$

$$\begin{aligned}
&= \rho \overline{\mathcal{C}\mathcal{C}} : \frac{\partial v}{\partial r} \\
&= P_k : \frac{\partial v}{\partial r}
\end{aligned} \tag{B-50}$$

$\overline{n\phi(\frac{1}{2}m\mathcal{C}^2)}_{coll}$ is split into three terms as follows [32]:

$$\overline{n\phi(\frac{1}{2}m\mathcal{C}^2)}_{coll} = -\frac{\partial q_{coll}}{\partial r} - P_{coll} : \frac{\partial v}{\partial r} + N(\frac{1}{2}m\mathcal{C}^2)_{coll} \tag{B-51}$$

where q_{coll} is the collisional granular heat flux, P_{coll} is the collisional stress tensor, and $N(\frac{1}{2}m\mathcal{C}^2)_{coll}$ is the energy from the inelastic collisions [31].

Substituting Equation B-46 to B-51 into B-45, the fluctuating energy equation is obtained as follows:

$$\frac{3}{2} \frac{D\rho\Theta}{Dt} + \frac{3}{2} \rho \Theta \nabla \cdot v + \frac{\partial q_k}{\partial r} + P_k : \frac{\partial v}{\partial r} = -\frac{\partial q_{coll}}{\partial r} - P_{coll} : \frac{\partial v}{\partial r} + N(\frac{1}{2}m\mathcal{C}^2)_{coll} \tag{B-52}$$

Rearranging the equation above gives:

$$\frac{3}{2} \frac{D\rho\Theta}{Dt} + \frac{3}{2} \rho \Theta \nabla \cdot v = -\left(\frac{\partial q_{coll}}{\partial r} + \frac{\partial q_k}{\partial r}\right) - (P_{coll} : \frac{\partial v}{\partial r} + P_k : \frac{\partial v}{\partial r}) + N(\frac{1}{2}m\mathcal{C}^2)_{coll} \tag{B-53}$$

$$\frac{3}{2} \frac{\partial \rho \Theta}{\partial t} + \frac{3}{2} v \cdot \frac{\partial \rho \Theta}{\partial r} + \frac{3}{2} \rho \Theta \nabla \cdot v = -\left(\frac{\partial q_{coll}}{\partial r} + \frac{\partial q_k}{\partial r}\right) - (P_{coll} : \frac{\partial v}{\partial r} + P_k : \frac{\partial v}{\partial r}) + N(\frac{1}{2}m\mathcal{C}^2)_{coll} \tag{B-54}$$

$$\frac{3}{2} \left[\frac{\partial \rho \Theta}{\partial t} + \nabla \cdot (v \rho \Theta) \right] = -\frac{\partial (q_{coll} + q_k)}{\partial r} - (P_{coll} + P_k) : \frac{\partial v}{\partial r} + N(\frac{1}{2}m\mathcal{C}^2)_{coll} \tag{B-55}$$

or

$$\frac{3}{2} \left[\frac{\partial \rho \Theta}{\partial t} + \nabla \cdot (v \rho \Theta) \right] = -\nabla \cdot (q_{coll} + q_k) - (P_{coll} + P_k) : \frac{\partial v}{\partial r} + \gamma \tag{B-56}$$

where $\gamma = N(\frac{1}{2}m\mathcal{C}^2)_{coll}$.

Recalling the definition of τ_s and letting $q = q_{coll} + q_k$, then the following equation is achieved:

$$\frac{3}{2} \left[\frac{\partial \rho \Theta}{\partial t} + \nabla \cdot (v \rho \Theta) \right] = -\nabla \cdot q + (\tau_s) : \frac{\partial v}{\partial r} + \gamma \tag{B-57}$$

Substituting Equation B-41 into Equation B-57, the following equation is achieved for multiphase flows:

$$\frac{3}{2} \left[\frac{\partial \alpha_s \rho_s \Theta}{\partial t} + \nabla \cdot (\alpha_s \rho_s \Theta v) \right] = -\nabla \cdot q + (\tau_s) : \frac{\partial v}{\partial r} + \gamma \tag{B-58}$$

Thus in order to solve Equation B-58 for the granular temperature Θ , the following equations were applied to model the unknown variables q , τ_s and γ [20, 23, 32, 131].

B.3 Energy Transport Equation

The derivation of energy equation starts from the following enthalpy change equation [26]:

$$\rho \frac{DH}{Dt} = -(\nabla \cdot q) - (\tau : v) + \frac{DP}{Dt} \quad (\text{B-59})$$

where H is the enthalpy, and q is the energy addition by heat conduction.

Consider enthalpy as a function of pressure and temperature, then,

$$\begin{aligned} dH &= \left(\frac{\partial H}{\partial T}\right)_P dT + \left(\frac{\partial H}{\partial P}\right)_T dP \\ &= C_p dT + \left(\frac{\partial H}{\partial P}\right)_T dP \end{aligned} \quad (\text{B-60})$$

And the differential form of enthalpy is defined as follows:

$$dH = TdS + VdP \quad (\text{B-61})$$

where V is volume and S is entropy

Divide both sides of Equation B-61 by dP at constant temperature

$$\left(\frac{\partial H}{\partial P}\right)_T = T\left(\frac{\partial S}{\partial P}\right)_T + V \quad (\text{B-62})$$

According to Maxwell Relations,

$$\left(\frac{\partial V}{\partial T}\right)_P = -\left(\frac{\partial S}{\partial P}\right)_T \quad (\text{B-63})$$

Substituting Equation B-63 into Equation B-62,

$$\left(\frac{\partial H}{\partial P}\right)_T = V - T\left(\frac{\partial V}{\partial T}\right)_P \quad (\text{B-64})$$

Substituting Equation B-64 into Equation B-60,

$$dH = C_p dT + [V - T\left(\frac{\partial V}{\partial T}\right)_P] dP \quad (\text{B-65})$$

Thus, the following equation is achieved:

$$\rho \frac{DH}{Dt} = \rho C_p \frac{DT}{Dt} + \rho [V - T\left(\frac{\partial V}{\partial T}\right)_P] \frac{DP}{Dt}$$

$$\begin{aligned}
&= \rho C_p \frac{DT}{Dt} + \rho \left[\frac{1}{\rho} - T \left(\frac{\partial \left(\frac{1}{\rho} \right)}{\partial T} \right)_P \right] \frac{DP}{Dt} \\
&= \rho C_p \frac{DT}{Dt} + \left[1 + \frac{T}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \right] \frac{DP}{Dt} \\
&= \rho C_p \frac{DT}{Dt} + \left[1 + \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_P \right] \frac{DP}{Dt}
\end{aligned} \tag{B-66}$$

Substituting Equation B-66 into Equation B-59 and rearranging the equation yields:

$$\rho C_p \frac{DT}{Dt} = -(\nabla \cdot q) - (\tau : \nabla v) - \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_P \frac{DP}{Dt} \tag{B-67}$$

The gases in the gasifier are assumed as ideal gases because the gasifier in this research is operated at atmospheric pressure. Thus, for an ideal gas, the gas density can be calculated as follows:

$$\rho = \frac{PM}{RT} \tag{B-68}$$

where M is molecular weight.

Thus, the last term in the RHS of Equation B-67,

$$\begin{aligned}
\left(\frac{\partial \ln \rho}{\partial \ln T} \right)_P &= \left[\frac{\partial (\ln PM - \ln RT)}{\partial \ln T} \right]_P \\
&= - \left[\frac{\partial (\ln R + \ln T)}{\partial \ln T} \right]_P = -1
\end{aligned} \tag{B-69}$$

According to Fourier's Law,

$$-\nabla \cdot q = \nabla \cdot (k \nabla T) \tag{B-70}$$

Substituting Equation B-69 and Equation B-70 into Equation B-67, the following equation is obtained:

$$\rho C_p \frac{DT}{Dt} = \nabla \cdot (k \nabla T) - (\tau : \nabla v) + \frac{DP}{Dt}$$

For heat conduction in turbulent flows, the thermal conductivity is replaced with the effective thermal conductivity, k_{eff} , defined as:

$$k_{eff} = k + \frac{C_p \mu_t}{Pr_t} \tag{B-71}$$

where Pr_t is the turbulent Prandtl number.